Developments in DESY's Photon Science Detector Group

High Resolution and High Rate X-ray Detec

Challenges from Photon Science Percival AGIPD High-Speed Imager

Cornelia Wunderer DESY Photon Science Detector Group VISTAS Workshop, Heidelberg, Sept 30-Oct 1 2019

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Photon Science is a very broad field

... from Fundamental Physics to Materials Science to Pharmacology ...

- e.g. Petra III Synchroton today supports 21 beamlines (more coming ...)
 - Bio-imaging
 - Chemical Crystallography
 - Materials Science
 - Spectro-micoscopy down to nanoscale
 - Extreme Conditions Research (pressure, temperature)
 - ...
- Free Electron lasers open new realms (high brilliance, ~10 fs timescales)
- European XFEL in Hamburg today supports 6 end stations, facility accommodates 12
- Science:
 - Molecular dynamics (how do chemical reactions evolve?)
 - Detailed studies of materials susceptible to radiation damage "outrun the damage by getting information out fast"
 -







Science at FELs: Shot-by-Shot imaging is key

- One textbook example: crystallography of single molecules or nanocrystals
 - Sample is literally vaporized by single FEL pulse
 - Individual FEL photon bunch is only 10s of femtoseconds
 - Diffraction occurs before molecule has time to disintegrate
 - Orientation of every individual sample is different
 - Diffraction of every sample must be imaged separately
 - Combining many thousands of diffraction patterns (of unknown orientation!)
 - Calculate structure of diffracting molecule
 - Example at right: Avibactam bound to beta-lactamase (1st structure solved in early experiments at Eu.XFEL)





Examples of images to be recorded at FELs

Even "just" from coherent diffraction imaging: large variety of X-ray images, no "common characteristics" apparent



Challenges of Today's Photon Sources

- Many FELs around the world today operate at 50-120Hz repetition rate
- **Superconducting FELs** (to date FLASH and European XFEL), for thermal reasons, operate in bursts of "pulse trains"
 - FLASH: 10 Hz base period, every 100ms a train of up to 800 pulses at 1MHz
 - Eu.XFEL: 10 Hz base period, every 100ms a train of up to 2700 pulses at 4.5 MHz
 - This basic machine property turns out to be very inconvenient for e.g. sample delivery, or detectors
- 3-rd generation synchrotrons are mostly used as "continuous light sources"
- In most imaging experiments, photon counting as opposed to chargeintegrating – detectors can be used (no more than one photon per pixel per pulse to be recorded)





Challenges of Future Photon Sources

Common denominator: imaging detectors with 100kHz+ continuous frame rate and high dynamic range required

- Diffraction-limited storage rings (Petra IV)
 - Reducing emittance by ~ factor 100 -> brilliance up by 2 orders of magnitude
 - Much-increased coherence
 - Detectors must keep up
 - Higher dynamic range, possibly more than one photon per pixel bunch
 - Faster experiments -> image readout at correspondingly higher rate
 - For some: photon timing down to single bunches (4ns spacing)
- ContinuousWave ("CW")-operation of superconducting-LINAC FELs (Eu.XFEL)
 - Motivated by less complex detectors & sample delivery (vs bursts of pulses)
 - Implies more dissipated heat -> more cooling needed by machine
 - Expect number of electrons / photons per second roughly as today
 - Bunch spacing in the 100kHz 1 MHz range expected (the larger the spacing, the more photons per bunch)
 - FELs require detectors capable of single-shot science -> drives frame rate





Percival

"Pixelated Energy Resolving CMOS Imager, Versatile And Large"



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Soft X-ray CMOS Imager for FLASH and Petra III: Percival

CMOS imager to meet the combination of challenges

- Novel imager meeting key FEL challenges simultaneously, in the soft X-ray regime:
 - (at least) Megapixels in a single sensor (avoid dead area)
 - fast enough for "shot by shot" science @ today's FELs
 - dynamically adjust to single photons & large signals
- Project initiated by DESY
- Actively invited collaboration from the community
 -> today five light sources plus RAL/STFC, DESY lead
- Sensor CMOS design at RAL, with tight feedback loops to DESY ASIC designers and system experts
- System overall design by DESY, with contributions from partners





Percival 2M Sensor

Designed by partner Rutherford Appleton Lab / STFC

- CMOS imager (180nm technology)
- On-chip digitization (11520 ADCs)
- 3 auto-adjusting gain levels (per pixel, per frame, overflow)
- 1408 × 1484 pixels, 27μm × 27μm
- 4 × 4 cm² continuous imaging area (stitched sensor)
- option: 13 Megapixel imager, 120 Hz, 10 × 10 cm²
- Data rate at 300Hz frame rate is 20 Gbit/s, streamed out over 45 LVDS lines (240 MHz, double data rate)



1408 x 1484 pixel P2M



Percival's auto-adjusting multiple gains

- Classic 3T pixel, expanded by switches & increasingly large capacitors for 3 gains & overflow
- · What are we trying to achieve?
 - To discriminate 1 photon from 0 we need noise floor 15e- or less (at 250eV one photon generates 69 e-)
 - 5*10⁴ photons -> 3.5 Me-
 - If 3.5 Me- correspond to 3.3V, 17e- would be ${\sim}15\mu V$... hard to measure, and we'd need too many bits
- Switches 0-2 set to ~0.7 V during integration, enabling a current to the adjacent larger capacitor/overflow only if large charge deposits have lowered the diode / smaller cap voltage to roughly this transistor gate voltage
- During readout, voltages on the diode, diode + 1st capacitor, ... probed sequentially
- one value (decision based on thresholds) converted by ADC



Post-processing of Sensors

Necessary to optimize performance for soft X-rays, UV light, as well as low-energy charged particles

- Attenuation lengths in Si / SiO2 at or below 100nm for soft X-rays
- Attenuation lengths for few-keV electrons in Si are on the order of 10s of nm
- Interaction must happen in active Si, and generated charge cloud must reach the circuitry

Requires:

- Negligible passive layer
- Negligible traps
- · Optimized geometry of electric field at surface of sensor



Attenuation Length of Photons in Si and SiO₂

Why work in this very challenging regime?

Science Challenges – two examples

- Water window offers unique view of biological systems: Between Carbon and Oxygen edges, water is transparent but carbon absorbs
- 282 eV to 533 eV photons



• Sweet spot for these measurements is around 500 eV electron energy (plus few keV acceleration from optics)

Imaging bio-systems



Soft X-rays

Ekberg et al. 2015

Molecular dynamics



PostProcessing of Sensors for soft X-ray performance

Optimal science use requires processing beyond foundry wafer production and 3D integration

Our science requires access to

- Flexible thinning capabilities for CMOS chips and wafers
- Surface post-processing for thin entrance windows & optimal electric fields
- Quick turnaround and flexible access for prototype development





Paths:

- Percival prototype: 1st generation wafer BSI-processed by JPL
- Percival 2M:
 - JPL key partner, will process wafers (1st done)
 - Exploring alternate routes to "good" post-processing in parallel – for some applications 10s of nm are acceptable
 - EMFT currently a partner in tests (bonding, thinning, pad exposure)
 - · Easier-to-access MBE-based post-processing for wafers and single dies (prototypes) would be very useful



The Percival 2M System

- DESY. In-vacuum detector head ٠
 - sensor ٠
 - Includes sensor biasing board DESY. .
 - Several hundred LVDS control & data ٠ DESY. lines, are (re)distributed here
 - Sensor will be cooled to ~ -30°C ٠
 - 2-side buttable ٠
 - movable •









LTCC routing & actual board

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The Percival 2M system

- Carrier board hosts
 - FPGA running finite state machine
 - Mezzanine board (also AGIPD, Lambda) reordering data for easier processing streaming out 20 Gbit/s data
 - Interface to slow control, facility information, trigger

- Control & DAQ
 - 20 Gbit/s from one sensor (reading full images: 300 Hz, 2M pixels, 30 bit/pixel incl. CDS)
 - Saving to standard format on disk (hdf5 with extensions)
 - Interface to standard control tools at beamlines

- Software Framework for Characterization
 - Data validation

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- Calibration constants
- Sensor characterization







Testing

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Stitched CMOS sensor in action: Percival 2-Megapixel "P2M"

- 4cm x 4cm stitched imaging area
- 1484x 1408 pixels, each 27 $\mu m \times 27 \ \mu m$
- P2M Power-up commenced in late September 2017, significant initial hurdles understanding ADC (crosstalk ...)
- P2M front illuminated version used for first experiments
- P2M first backside-illuminated version tested successfully, however without the processing required for high soft X-ray QE
- P2M with JPL's delta doping currently being wirebonded
- First JPL-processed P2M to see soft X-rays in Dec 2019



P2M first (visible) light image (Dec 2017), top left: prototype image on same scale

Using first Percival P2M (front-illuminated version)

Here with a scintillator coupled to the sensor, for imaging with harder X-rays at Elettra

- Coupling thin scintillator to FSI sensor at Elettra
- Tomography of a mouse's head



credits to G. Pinaroli (now BNL), G. Lautizi, S. Donato, and R. Menk



Percival Prototype Performance

BSI-processed early prototype

 Imaging at 92 eV, single-shot at FLASH

left: Airy ring pattern

right: fine diffraction rings from liquid sample

- Airy rings match expectation
- Charge Collection Efficiency (lower limit to quantum efficiency) measured at ~70% above 400eV



Performance of first Percival P2M (front-illuminated version)



- Gain switching demonstrated to work
- Tender X-ray beam imaged illustrating auto-adjusting gains



Performance of first Percival P2M (front-illuminated version)

- Noise: <16e- noise demonstrated
- so far operation at 83Hz for full sensor Speed: DAQ timing issues cause factor 2 reduction today's crosstalk workaround -> another factor 2
- Full Well : > 3.5 Me- (more than 5e4 ph @ 250eV)
- P04 beamline (Petra III), end of 2018: 800 First tender X-ray images on FSI 700 1-photon 600 sensor only ocurrences coarselv tuned 500 2-photons 400 300 3-photons 200 Thanks to P04 staff for support! 100 0 0 50 100 150 200 250 pixel output [ADU] head FSI01 noise (T-20, PGA6, CMS-CMA, H0) 25 20 **je [e]** 15 þ. ά ¢. ¢. ¢. 10

20

40

60

t_{int} [ms]

80

pix(317,536), CDS-CMA

- Tuning the system is still in progress: .
 - Complex firmware change required to circumvent on-chip crosstalk. until this is implemented low-noise mode (linear ADC behavior with <16e- noise) only accessible on 3/7 rows
 - Full-sensor readout images with • today's firmware carries higher noise or requires handling non-linear ADC response





100

AGIPD – new developments

Hybrid multi-megapixel imager developed for the European XFEL 2nd generation systems

- compact readout for 4-Megapixel array
- electron-detecting AGIPD for high-Z sensors











AGIPD in a Nutshell

1Mpix systems, installed and operating at SPB/SFX (since 2017) and MID (2018)

Main features:

- High dynamic range:10⁴ photons/(shot*pixel) at 12.4 keV photon energy
- Single photon sensitivity (σ_{noise} = ~1keV)
- High frame rate (4.5 MHz, matches X-ray intra-train rep. rate)
- External veto capability
- Sensor: Silicon, thickness 500 μm
- Pixel size: 200 μm x 200 μm

AGIPD is a Hybrid pixel array detector

- Diode detection Layer (Sensor)
 - Fully depleted, high resistivity
 - Direct X-ray conversion
 - Silicon, GaAs, CdTe, etc
- Connection Bump Bonds
 Solder or Indium, 1 per pixel
- CMOS Layer (Application Specific Integrated Circuit ASIC) signal processing, storage, output
- Sensor & ASIC designed independently => large flexibility

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AGIPD 1.1 ASIC



Remaining Issue: Separation between med/low gain signals disappearing with burst length → AGIPD 1.2



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AGIPD 1Mpix Systems:

... calibration is a real challenge!

Feed calibration framework with

- Pulsed capacitor dynamic range scans for all memory cells used
- $Cu-K_{\alpha}$ data at XFEL
- Dark data for High and Medium gain level





- 65,536 pixels (x 16 modules)
- 352 memory cells
- 3 Gains + 3 Offsets
- ≈138,000,000 fits / module
- 16 Modules $\rightarrow 2.2 \times 10^9$ constants



computation time, fit quality, non-constant fit ranges



- In-vacuum z-motion
 through gate valve (inner diameter 800mm)
 into sample chamber
 - travel range of 400 mm

- Two halves
 - 2 x 14 modules each
 - Independent in-vacuum x-motion









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In-vacuum cooling



AGIPD 1M Detector for HiBEF

@HED Endstation of European XFEL





The HiBEF (Helmholtz International Beamline for Extreme Fields) experiment @ EuXFEL needs a 1Mpix detector for **E**_{ph}**25keV**

- The existing AGIPD detector collects positive charges (holes)
 - Easier to realise radiation hard sensors
 - Slower less demanding to handle large charges (circuit wise)
- AGIPD is not suitable for experiments with photons above ~15keV (Silicon sensor inefficient above ~15keV)
- High-Z Semiconductors, esp. GaAs, promise efficient sensors for E_{ph} ≥ 25keV
- Composite (III/V) Semiconductors feature relatively short charge carrier lifetimes
- Collection of Electrons (i.e. the fast component) is required

=> new ASIC needed! *ecAGIPD,* prototype AGIPD06 showed promising performance

New AGIPD sensors for higher energies

HIBEF: photon energies 20-30 keV

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- Requires "heavier" (high-Z) materials
- Experience with these exists from Lambda (Medipix) Systems
- Germanium (Ge) very difficult due to high cooling requirements (narrow bandgap Eg=0.74 eV @ 0 K)
- GaAs from Tomsk State University, Inhouse test systems: 500 mm, ohmic-type contacts, single-ASIC size, AGIPD 1.1 hole-collecting
- CdTe from Acrorad Inhouse test systems: 750 mm, Schottky-type contacts, single-ASIC size, ¹/₂-FEM size, AGIPD 1.1 hole-collecting
- CdZnTe, from Redlen Technologies, ordered
- with ecAGIPD, better-adapted test systems will be possible





E. Hamann et al., IEEE Transactions on Medical Imaging 34, No. 3, 2015



High-Speed-Imager

Answering the future challenges inherent to both CW-operation of Eu.XFEL, and diffraction-limited storage rings such as Petra IV

- * Continuous imaging at ≥ 100 kHz pulse repetition rate
- * High dynamic range



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Wish List for a high-speed imager

Conceptual design currently being developed

- ≥ 100 kHz continuous frame rate
- Multi-megapixel (>10 Mpixel)
 - Minimal dead area
- ≤ 100 µm pixel size
- Single photon sensitivity
- 10⁵ photon upper range
 - Noise below Poisson statistics
- Compatible with different sensors for hard / soft X-rays
- Compatible with vacuum operation
- Radiation hard

Conceptual Design Report for a 100+ kHz X-ray imager

David Pennicard, Ulrich Trunk, Sergej Smoljanin, Heinz Graafsma - DESY

Introduction

This document presents a Conceptual Design for a "Very High Frame-Rate" X-ray imager. It starts with the scientific justification of the need for such a system, which is only meant to give a background so as to better understand the requirements in the subsequent section. It is to be understood that these requirements are not set in stone and some, but not all, can be relaxed. Also since this is a project under development, some requirements might get even stricter. Some requirements might turn out to be mutually exclusive, in which case a compromise will need to be made.

The main part of the document gives a description of the system components, their specifications, and potential solutions, with the goal to make sure that such a system can actually be built with realistic resources and within an acceptable time. This document is a first step in a process and it might be advantageous, at some time, to organize a limited-sized workshop, with invited experts in specific areas. The goal of the process is to arrive at a comprehensive project plan, possibly via a Technical Design Report. The goal is to have the technical design and the comprehensive project plan ready by the end of 2018.

Justification for a 100+ kHz X-ray imager

The European XFEL currently runs in its unique burst-mode, with up to 2700 pulses in 0.6 milli-seconds, repeated 10 times per second. This does produces 27 000 pulses per second, which is significantly more than any other FEL source in the world. However, this burstmode of operation is sub-optimal for many experiments, and a more uniform distribution of pulses over time (often called Continuous Wave, or CW) would be more profitable. At the same time other FELs, noteably LCLS, are in the process of implementing high-repetition CW operations, with up to 1 MHz rep rates. As a natural development, also the European XFEL will eventually provide CW-mode operation options. The current plans foressee different modes of operation, including the current burst-mode, termed short (RF-)<u>pulse</u>, a mode with 50% duty cycle, termed long pulse, and a CW mode. The total number of pulses in each mode is still to be determined, but the total current in the machine will stay more or less the same. This means in retrun that the total number of pulses per second can only be increased by lowering the charge per bunch. Lowering the bunch charge by a factor of 4, would give about 100 000 pulses per second. In CW they would be equally spaced, in the long pulse mode, they would be a factor 2 closer spaced, giving 200 KHz repetition rate.

AT the same time PETRA III is, almost certainly, being upgraded to a Diffraction Limited Storage Ring (DLSR). This will result in an increase in brilliance by a factor of around 100 (less for soft X-rays, more for hard X-rays), so experiments previously performed at kHz frame rates

High Frame Rate Integrating ASIC design?



Key Challenges to address

Dynamic range, and analog-to-digital conversion

- Dynamic range larger than AGIPD's, in smaller pixels
 - Putting a large capacitor in the pixel won't be enough (limit few 10⁴ ph/pixel/frame at 12 keV even with combined cap types)
 - Alternative approaches and ideas needed
 - Read out of "charge batches" during integration (compare MMPAD from Cornell)?
 - Measure/split overflow current in some way (compare FASPAX from Fermilab)?
 - ...

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- Analog-to-digital Conversion, AGIPD Model: Analog readout & conversion off-chip
 - For AGIPD, 1024 pixels per output line running @ 33MHz, 16 kHz frame rate operation works
 - Analog transmission becomes very delicate above few 10MHz
 - · Conversely, digital transmission is not a problem
 - Off-chip conversion is NO-GO => must digitize on-chip





Key Challenges to address

Converting analog pixel data to digital values - and Power needs of the ASIC

- Digital conversion on-chip, <100um pixels at 100+kHz rate
 - DSSC: 5MHz, 8-bit single-slope ADC in ~ 1/3 of 200um pixel (130nm CMOS)
 - Pixfel design papers: 5MHz, 10-bit SAR ADC in 97um x70um (65nm CMOS)
 - Sharing ADC between multiple pixels?
 - e.g. 4x 100um pixel @ 1MHz, or 16x50um pixel at 250kHz?
 - Achieving the desired dynamic range, below Poisson noise limit & with a limited number of gains, would be more comfortable with 12 bit ...

ASIC Power

- Dynamic gain switching
- Pixel size 50µm...500µm
- Digitization with 16 bits
- at a frame rate of 1kHz 500kHz
- Assumption: P=200µW+500pW/Hz



PIXFEL pixel layout (from PhD thesis L.Lodola 2016)



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Key challenges to address

Speed limits from power, & data throughput

Data rate off ASIC

- Options exist, though pushing the limits
 - Samtec FireFly offers 28Gbit/s/link; 24Gbit/s/link (net); 12 links/unit
 -> taking footprint into account: 48Gbit/s/cm2
 - LpGBT (CERN development) may be another way to get data off the ASIC
- DAQ and analysis become "Big Data" challenges

Data rate out of the front-end

- 100kHz x 1M pix of 100umx100um pixels x 10-12 bit ADC + 2bit gain 12-14 bit x 100 GHz from 10 cm x 10cm, or ~200 Gbyte/s from 10cm x 10cm,
- scientists want to instrument several Megapixels in an experiment, so
 - we're talking multi-Tbyte/s from the detector
 - the back end must fit within the footprint of the sensor to be tileable





Key Challenges

Readout architecture options

- Route digital outputs of chips to specialized transceivers on FPFA
- Serialize data, and transmit on high-speed optical links
- One example: 900Gbit from a 10cm x 2.5cm module, with 100um pixels at 300kHz frame rate



- Less efficient bandwidth usage of links
 (limited by chip transceivers)
- Must use specialized transceiver board (however note FPGA power desired at that point anyways for image conversion etc)



Readout board

Chip (130 nm)

Key Challenges

What to do with the data once it's off the sensor?

- 200 Gbyte/s from 1Mpix, expect 10Mpix systems in use -> 2Tbyte/s
- How **to reliably receive data** from the detector at this rate? (expect today's approach of using Linux network stack may not work ...)
- · Convert raw ADUs to photon images in real time
 - FPGA-based approach?
 - GPUs an option?
- Data reduction & rejection of bad images
 - Fairly simple first examples in photon science could be
 - Rejection of images where no sample was hit (needs view of full image!)
 - Simple compression schemes such as efficient encoding of zeroes
 - Highly experiment-specific => much more complex than in particle physics!
 - Photon science will have to learn ...





Summary and Conclusions

- Photon Science provides unique and ever-evolving challenges to detector developers ranging from sensor physics to electronics to system engineering to mining big data
- Photon sources are a big driver of detector needs *future ballpark 10Mpix+ at 100kHz+ and 10^5-10^6 dynamic range*
- · Data reduction schemes will soon become mandatory

• AGIPD:

- First 1M systems are a success story
- Evolution into larger (4M), more compact (new readout) systems with broad sensor range (e-collecting for high-Z/HIBEF)

• Percival:

- Understanding a large sensor can take time (in our case: overcoming crosstalk hampering on-chip ADC functionality by changed readout timing)
- Percival 2M 4x4cm2 imager works, in FSI configuration first "user images" taken with scintillator
- Percival 2M in BSI configuration with soft X-ray-compatible entrance window ready to power up as of Friday

(... stay tuned)

- High-speed imager
 - Detailed design being developed, options and tradeoffs being investigated
 - ASIC itself as well as backend (and cooling) present fundamental challenges



DESY's Photon Science Detector Group

Core task: ensure that Photon Science at DESY has the detectors needed for cutting-edge experiments (buy / collaborate / develop)



- ~ 25 people
- scientists, postdocs, mechanical & electrical engineers incl. FPGA expertise
- ASIC design in the group, some CMOS design expertise in the group
- All expertise needed for full (beamline) detector system within the group
- Spinoff founded a few years back: XSpectrum

There are open positions for PostDocs and Master/PhD students!

http://photon-science.desy.de/research/technical_groups/detectors/index_eng.html

Thanks

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