Towards the perfect imager: Detector developments for next generation X-ray sources

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Overview DESY

Particle Physics

Accelerators

Common Infrastructure

Light sources
- PETRA III (14 BL)
- DORIS III (31 BL)
- FLASH (5 BL)
- European XFEL

Photon science
- > 280 people
- > 2000 users/year

Partners
- CFEL
- GFZ Helmholtz Centre Potsdam
- EMBL
- Max-Planck Unit for Structural Molecular Biology
- The Helmholtz-Zentrum Geesthacht
- University of Hamburg
Overview

➢ Introduction to our group: DESY FS-DS

➢ Our projects for synchrotron radiation detectors
  ▪ LAMBDA project (new photon counting detector)
  ▪ High-Z pixel detectors (hard X-ray detectors)
  ▪ PERCIVAL project (new low energy detector)

➢ The European XFEL
  ▪ AGIPD project (new integrating detector for XFEL)

➢ Science example: XPCS@XFEL
Our group: DESY FS-DS

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Our detector development projects

- LAMBDA (Large Area Medipix3-Based Detector Array)
  - Photon counting pixel detector module

- High-Z detectors (HiZpad collaboration)
  - New semiconductor pixel detectors for hard X-rays

- PERCIVAL (Pixelated Energy Resolving CMOS Imager, Versatile And Large)
  - Low E (250 eV – 1 keV) imaging detector produced by STFC, readout by DESY

- AGIPD (Adaptive Gain Integrating Pixel Detector)
  - 2D detector for XFEL, developed with PSI, Uni Hamburg, Uni Bonn

- DSSC (DEPMOS Sensor with Signal Compression)
  - XFEL detector project, led by MPI-HLL, Munich
Other involvements

- CAMP (CFEL-ASG Multi-Purpose) Chamber
  - Already in use at LCLS
- Detector and science simulation (HORUS)
- Diamond beam position monitors with RF readout
  - Collaboration with ESRF
- Detector loan pool
  - Pool of a variety of detectors (Pilatus, Maxipix, CCDs, imaging plates, etc.) and associated equipment to support user operation at photon sources.
Hybrid pixel detectors (counting)

- Pixellated photodiode sensor
- Readout chip with 1 readout channel per pixel
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Hybrid pixels and X-ray detection

> First generation of X-ray hybrid pixels in use
  - Pilatus (Dectris, PSI)
  - Maxipix (ESRF, Medipix2 collaboration)

> Advantages
  - Single photon counting ("noise free")
  - Fast readout
  - Large dynamic range
  - Energy discrimination

> Disadvantages
  - Pixel-to-pixel variation in electronics (must be calibrated)
  - Poor efficiency at high energies
  - Problems at high flux rates
Detector developments at DESY

> Large Area Medipix-Based Detector Array (LAMBDA)
  - Large detector modules using new Medipix3 chip
  - Small pixel size, fast readout, greater functionality

> “High-Z” semiconductors
  - Si has poor absorption efficiency > 20 keV
  - Heavier semiconductors (Ge, CdTe, GaAs) allow hard X-ray detection

> PERCIVAL (Pixelated Energy Resolving CMOS Imager, Versatile And Large)
  - Low E (250 eV – 1 keV) imaging detector produced by STFC, readout by DESY

> Adaptive Gain Integrating Pixel Detector (AGIPD)
  - Integrating Detector with gain switching
  - In-pixel storage for ultra fast imaging at XFEL
Medipix3 readout chip

> 21 groups in collaboration
  ▪ Chip design at CERN
> Successor to Medipix2 (Maxipix)
> 256 * 256 pixels, 55µm
> 2 counters per pixel for deadtime-free readout
  ▪ Up to 2000 fps with 12 bit counter depth
> “Charge summing” circuitry to compensate charge sharing effects
  ▪ More reliable hit detection
  ▪ Better energy discrimination
LAMBDA detector head

> Large sensor area
  - 2-by-6-chip layout
  - 1536*512 pixel, 84 mm * 28 mm
  - Set by typical silicon and high-Z wafer sizes (6”, 3”)

> Suitable for high-speed readout

> Low-temp operation possible

> Modular design
  - Multiple readout chips build a single module
  - Multiple modules tiled in large system

1 large Si sensor
84 mm * 28 mm
or
2 “hexa” high-Z sensors
Each 42 mm * 28 mm

Voltage reg. board

500-pin high density connector
First prototype systems

- 4 modules built with “quad” sensors (2*2 chip, 512*512 pixels)
- Mechanics with Peltier cooling
- Electronics to one side of sensor (but right-angle connector now available)
- Prototype readout board (completed)
  - USB2 communication with control PC (10 frames per second with large-area sensor should be possible)
- High-speed readout
  - Common readout mezzanine board being developed for LAMBDA, PERCIVAL and AGIPD
  - Multiple 10 Gigabit Ethernet links for full-speed readout
Test results so far

- Detectors are working
  - Minor improvements needed to detector powering
- Currently working on full-size sensor and high-speed readout
Replacing Si with high-Z material could combine hybrid pixel advantages with high efficiency with hard X-rays

However, each high-Z material has its downsides!

Our projects:
- Germanium – development with Canberra and IZM (Berlin)
- Cadmium Telluride – HiZPAD consortium (led by ESRF)
- Gallium Arsenide – Russian-German partnership with FMF, KIT, JINR (Dubna) and RID Ltd. (Tomsk)

MAR345 ~2% at 100keV
Germanium sensor production and bump bonding

Sensor structure (Canberra)
- Modification of existing strip detector technology
- 55µm pixels, 700 µm thick

Indium bump bonding (IZM)
- Sensor and ASIC bonded at T < 100C
- During cooling, ductility of Indium compensates for mismatch in contraction

2 high purity Ge wafers plus mechanical dummies received from Canberra
- 16 Medipix3 singles / wafer
- IZM optimizing process using dummies
- HP Ge bonding follows soon

Readout and mechanics by DESY (LAMDA framework)
Cadmium Telluride

> HiZPAD (High-Z sensors for Pixel Array Detectors)
  - EU-funded consortium – 12 institutes (led by ESRF)

> CdTe ($Z_{\text{Cd,Te}} = 48, 52, Z_{\text{Si}} = 14$)
  - Already used in single-element detectors / small arrays
  - Small wafers (3”), often with inhomogeneities

> Tested CdTe sensor with Medipix2 readout
  - 55µm pixel, 256 * 256 array, 1000 µm thick
  - Tests done at DORIS III - BW5 beam line (160 keV photons)
PERCIVAL project

Aspired performance parameters:

- Primary energy range 250 eV – 1 keV (will work from <200 eV to few keV)
- 12 µm Si sensitive volume with 25 µm pixels ⇒ 4k × 4k pixel sensor
- 4 sensors in cloverleaf arrangement can make up 64 Mpixel (20cm × 20cm)
- back-illuminated, back-thinned for uniform QE > 90%
- 120 Hz frame rate and lower
- 2-side buttable (space between active pixel edges on the order of 1mm)
- electronic noise < 15e-, “full well” ~ 20 Me-
- Multi-gain approach to access full dynamic range, all gains active all the time
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➢ Science example: XPCS@XFEL
17.5 GeV linear electron accelerator producing 12.4 keV x-rays (tunable) through FEL process
unprecedented peak brilliance
user facility: common infrastructure shared by many experiments
What can be done at an XFEL?

- **Imaging of tiny structures**
  - single bio-molecule imaging (or small crystals)
  - investigation of nanostructures

- **Imaging of ultra fast processes**
  - filming of chemical reactions
  - imaging of changes in magnetization states

- **Investigation of extreme states**
  - highly ionized states in matter
  - non-linear interaction of x-rays with each other or other photons
  - creation of extremely high pressure/temperature
Single shot imaging...

**e.g. Coherent Diffractive Imaging (CDI or CXI):**

![Diagram showing the process of Coherent Diffractive Imaging](image)

- **Particle injection**
- **10 fs pulse**
- **Solve the well known Phase Problem**
- **Noisy diffraction pattern**
- **Combine 10^5-10^7 measurements**
- **Classification**
- **Averaging**
- **Orientation**
- **Reconstruction**

...and data reconstruction

Phase reconstruction algorithms to reconstruct real space image
e.g. two cowboys and the sun:

K. J. Gaffney and H. N. Chapman,
Science 8 June 2007

real space image
diffraction image
reconstructed real space image

J. Becker, Cornell Seminar

2/17/12
Special structure of pulse trains:

• 600 µs long pulse trains at a repetition rate of 10 Hz
• Each train consists of 2700 pulses with a separation of 220 ns
• Each (SASE) pulse consists of $\approx 10^{12}$ photons arriving <100 fs

Beam energy:

• 5 – 25 keV (depends on station)
• 12.4 keV ($\lambda=0.1$ nm) nominal design energy for AGIPD
XFEL Detector requirements

- Dynamic range: $>10^4$
- Low noise
- Single photon sensitivity
- Radiation Hardness
- 4.5 MHz

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XFEL Detector projects

Three 2D-Detector consortia:

- **LPD** (Large Pixel Detector)
  - 500x500 µm² pixels
  - “gapless”
  - 3 gains in parallel

- **DSSC** (DEPMOS Sensor with Signal Compression)
  - hexagonal pixels
  - very low noise
  - non-linear gain

- **AGIPD** (Adaptive Gain Integrating Pixel Detector)
  - 200x200 µm² pixels
  - central hole
  - adaptive gain switching

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## XFEL challenges

### XFEL provides

- Simultaneous deposition of all photons

  - $10^{12}$ X-ray photons in <100 fs

### Challenges

- Single photon counting not possible
- Dynamic range: $10^4$ photons/pixel with single photon sensitivity

### Approach

- Charge integration
- Dynamic gain switching
  - 3 gain stages
  - Single photon sensitivity in highest gain

- High number of bunches

  - 2700 bunches per train (600 µs)

- Reading out of single frames during pulse train impossible

- Analog memory in the pixel using the $\approx 350$ storage cells per pixel
Imaging with AGIPD 0.2 prototype
**Specifications:**

- 1 Mpixel
- 4 quadrants
- 4 modules per quadrant

→ 1 module: 8 x 2 chips,
→ 1 chip: 64 x 64 pixels

- 200 x 200 $\mu$m$^2$ pixel size
- 500 $\mu$m silicon sensor
- Hole for direct beam
- Upgradable to 4 Mpix
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• Science example: XPCS@XFEL
Scattering on many particles

X-rays

Disordered sample

Acts like optical grating

Incoherent beam

Encodes average properties of the particles

Coherent beam

Additionally encodes position of each particle as ‘speckles’ on the average value

Changes in the positions of the scattering particles change the positions of the speckles
How XPCS is performed

• Probe sample sequentially with non-destructive XFEL pulses
• Analyze image series using intensity autocorrelation ($g_2$ function)
• Functional form determined by interaction mechanism
• Extract time constant

Non-destructiveness requires large low intensity XFEL pulses
-> resulting speckles will be small
The ‘gap’ in accessible time scale

Split and delay technique

Limited by propagation delay (distance)

Sequential XPCS

Limited by detector readout speed and flux

XFEL train length

Detector performance?

relevant timescale

Examples:

1 ps

1 ns

1 μs

1 ms

1 s

Diffusive atomic motion

Fast dynamics in colloids, alloys etc.

Slow dynamics in colloids, alloys etc.

Dynamics of small clusters

Dynamics of small particles, large clusters

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Detector requirements for XPCS

- 4 µrad angular resolution
  → 40 µm pixel size at 10m distance

  X AGIPD Pixel size is 200 µm

- Single photon sensitivity
  ✓ Provided by AGIPD

- Very high frame rate
  ✓ Single pulse imaging possible with AGIPD

- Acquisition of image sequence
  ✓ More than 350 images stored per train
Key simulation parameters

AGIPD storage is limited to 350 of 2700 frames. What is the best sampling scheme?

- Linear sequence of 350 images
- 350 logarithmic samples of 2700 pulses
- Realistic Q dependence due to 3D real space model
XPCS SNR (not photon SNR!)

4 regions identified:

A) Saturation $\propto \sqrt{Q}$

B) ‘Better than expected’

C) Non saturated high intensity results of first study

D) Low intensity results of first study / analytic expression

Oscillations due to intensity variations (form factor) not noise!

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Relative performance penalty

Simulations show penalty not as big as expected, but still no benefit

Analytic XPCS SNR considerations show no benefit
Relative error on relaxation rate

Compared to linear scheme the log scheme provides:

Access to secondary dynamics due to larger time base

Lower errors for slow dynamics (low Q)

Larger errors for fast dynamics (large Q)
‘Measurement’ results of diffusion constant are equal within their respective errors. Errors for lin/log sampling are similar (for this sample).
• XPCS insensitive to FEL fluctuations (not shown)
• Logarithmic sampling advantageous for studies of ‘slower’ dynamics (low Q, \( \tau \approx 1 \, ms \))
• Linear sampling advantageous for studies of ‘faster’ dynamics (high Q, \( \tau \approx 1 \, \mu s \))
Summary

- Exciting new projects
  - LAMBDAA (large area modules, 55 µm pixels, 2 kHz frame rate)
  - HiZ (Direct detection imaging at high energies)
  - PERCIVAL (low energy imaging with 25 µm pixels)
  - AGIPD (4.5 Mhz imaging at XFEL)

- Exciting new opportunities at XFEL
  - Extremely fast (<100 fs pulse duration)
  - Extremely bright (single molecule diffraction)
  - Extremely challenging
Backup
What is XPCS?

- Investigation of fluctuations in diffraction images
- Scientific case XPCS@XFEL: molecular dynamics in fluids, charge & spin dynamics in crystalline materials, atomic diffusion, phonons, pump-probe XPCS
The signal to noise ratio is derived from the dispersion of $g_2$ values (blue arrow)

$$SNR \overset{\text{def}}{=} \frac{g_2 - 1}{\text{err}(g_2)}$$

The relative error of the correlation constant is the error of fit result (violet arrow)
Calculate intensity autocorrelation function \((g_2)\) per pixel

Sequential mode (constant \(\Delta t\) between frames)

\[
g_2(n, k) = \frac{1}{F - k} \frac{1}{\langle I_n \rangle^2} \sum_{i=1}^{F-k} I_n(t_i)I_n(t_i + k\Delta t)
\]

- \(n\): number of the individual pixel, identifying Q vector \(Q(n)\)
- \(k\): integer number, identifying lag time \(\tau = k\Delta t\)
- \(F\): number of acquired frames
- \(\langle I_n \rangle\): average (over all frames) pixel value
DAQ architecture

- Front End Electronics (FEE)
- Front End Interface (FEI)
  - interface to Train Builder
  - integrated in 2D
- Train builder layer
  - builds trains
  - simple data processing
- PC layer
  - interface to cache
  - additional train building
  - more complex data processing
- Data cache
  - hold, analyze, reduce and reject data
  - post processing
  - commit to silo

C. Youngman, S. Esanov