MM-PAD-2.1: a detector for high-flux, wide-dynamic-range synchrotron studies up to 10 kHz

Kate Shanks
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Acknowledgements

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- **Cornell detector group, past and present:** Sol Gruner, Julia Thom-Levy, Mark Tate, Hugh Philipp, Divya Gadkari, Dan Schuette, Prafull Purohit, Marty Novak, Lena Franklin, and others…

- **Argonne MM-PAD-2.1 collaborators:** Nino Miceli, John Weizeorick, Jon Baldwin

- **Power users and guinea pigs:** Todd Hufnagel (Johns Hopkins), Krzysztof Gofryk (INL), Zahir Islam (ANL), Darren Pagan (Penn State)

- **CHESS colleagues and diffraction afficionados:** Kelly Nygren, Sven Gustafson

Takeaways

Wide-dynamic-range area detectors are critically needed at synchrotron beamlines in order to advance diffraction-based techniques – especially for dynamic studies.

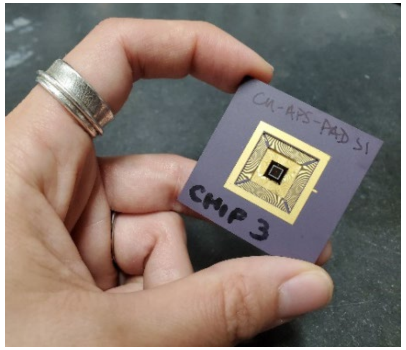
High-energy diffraction microscopy (aka 3DXRD) is a prime example of an application requiring increased dynamic range.

The **MM-PAD family** of detectors fills a unique “middle ground” combining key benefits of photon-integrating and photon-counting architectures.

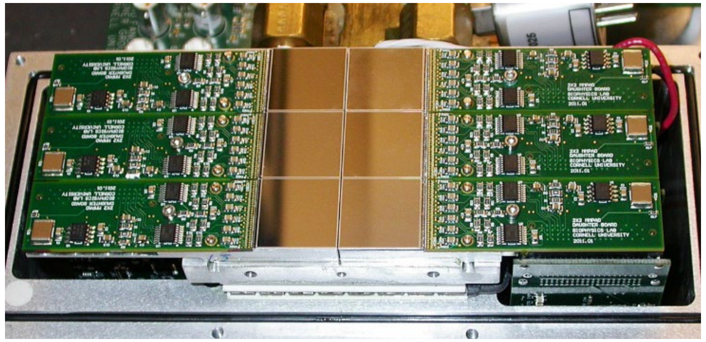
Increases to dynamic range + frame rate must be accompanied by new strategies for managing **large data volumes** and **high data rates**.

Detector R&D at Cornell

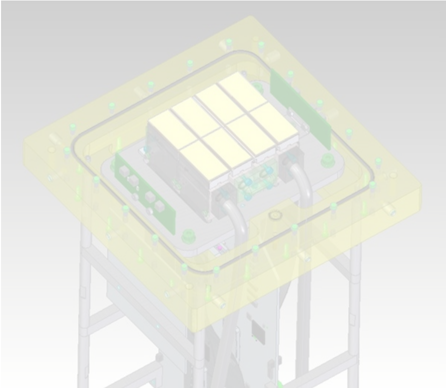
Our typical development cycle:



Small-scale modules for pixel design

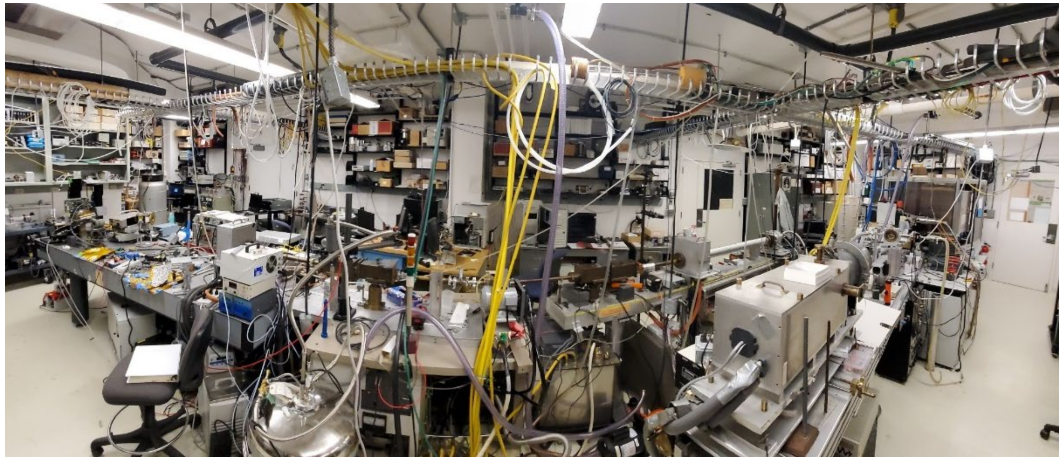


Medium-scale lab prototypes

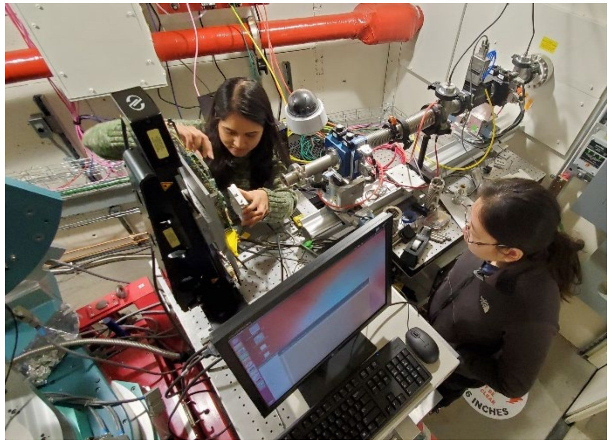


Tech transfer to commercial partners

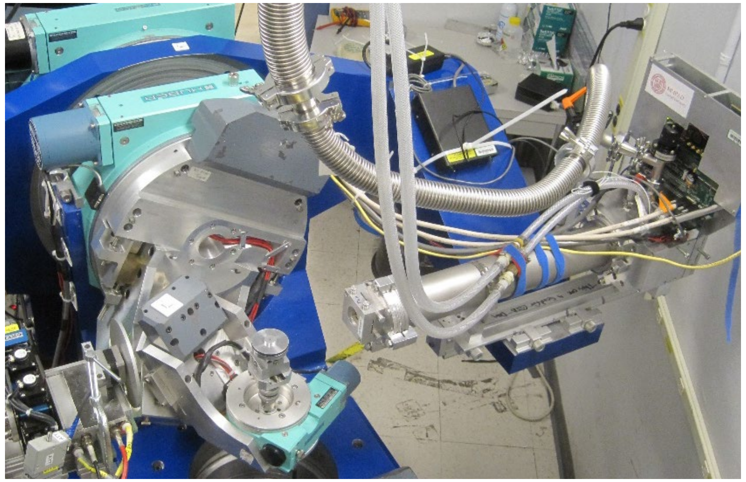
Detector proving grounds:



Characterization with home-lab sources



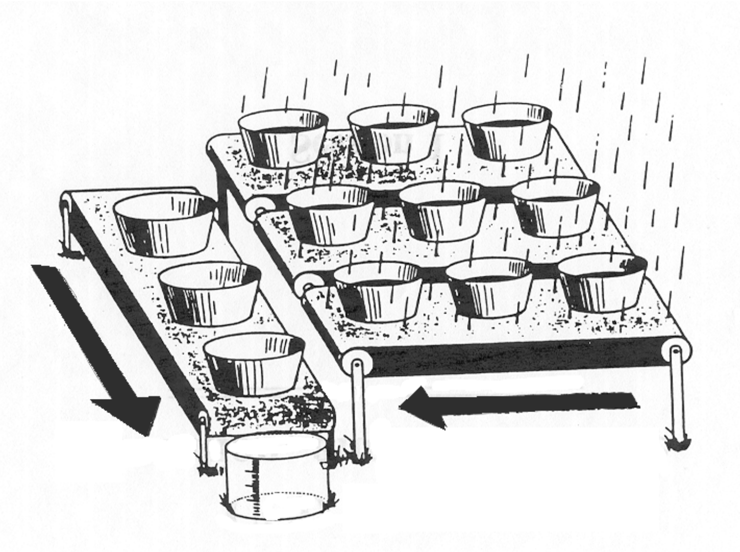
Characterization @ the beamline



User experiments @ the beamline

Photon integrating vs. counting

The canonical slide



Integrating

- Pixel well determined by size of bucket (typical: ~10^2 - 10^4 photons)
- Read noise, dark current present
- No inherent photon rate limit

Counting

- Pixel well determined by size of counter (>> 10^4 photons)
- Read noise, dark current suppressed
- Photon rate limit ~10^6 ph/pix/s

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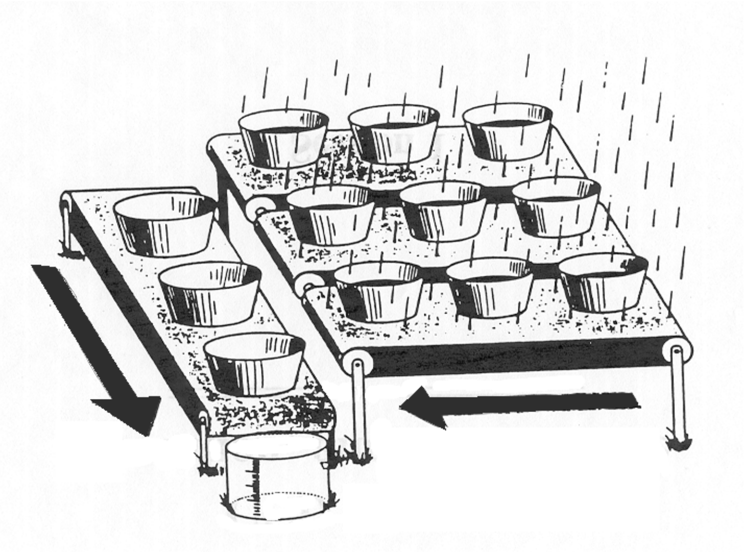

Integrating

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Why do we care?

Counting

- Pixel well determined by size of counter (>> 10^4 photons)
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- Photon rate limit ~10^6 ph/pix/s

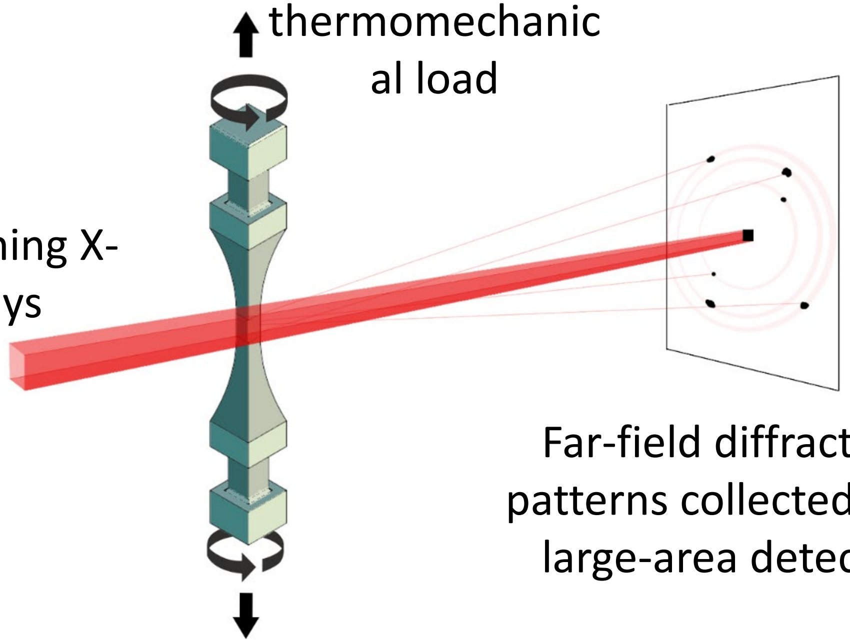
Let's consider a specific use case…

High-energy diffraction microscopy / 3DXRD

Rotation-based diffraction technique using *isolated diffraction spots* from a polycrystalline sample to reconstruct the **centroid, strain tensor, and orientation** of individual grains

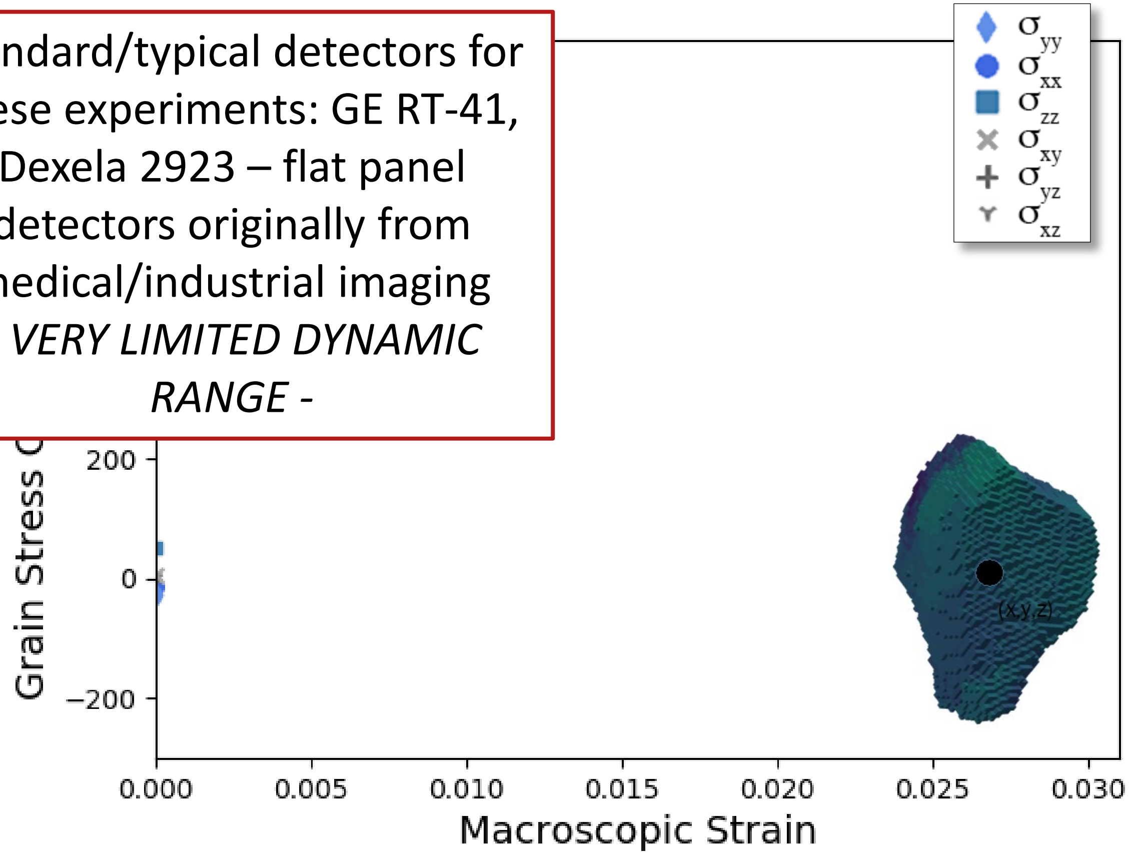
Sample under thermomechanical load

Incoming X-rays



Far-field diffraction patterns collected on a large-area detector

Standard/typical detectors for these experiments: GE RT-41, Dexela 2923 – flat panel detectors originally from medical/industrial imaging
- *VERY LIMITED DYNAMIC RANGE* -

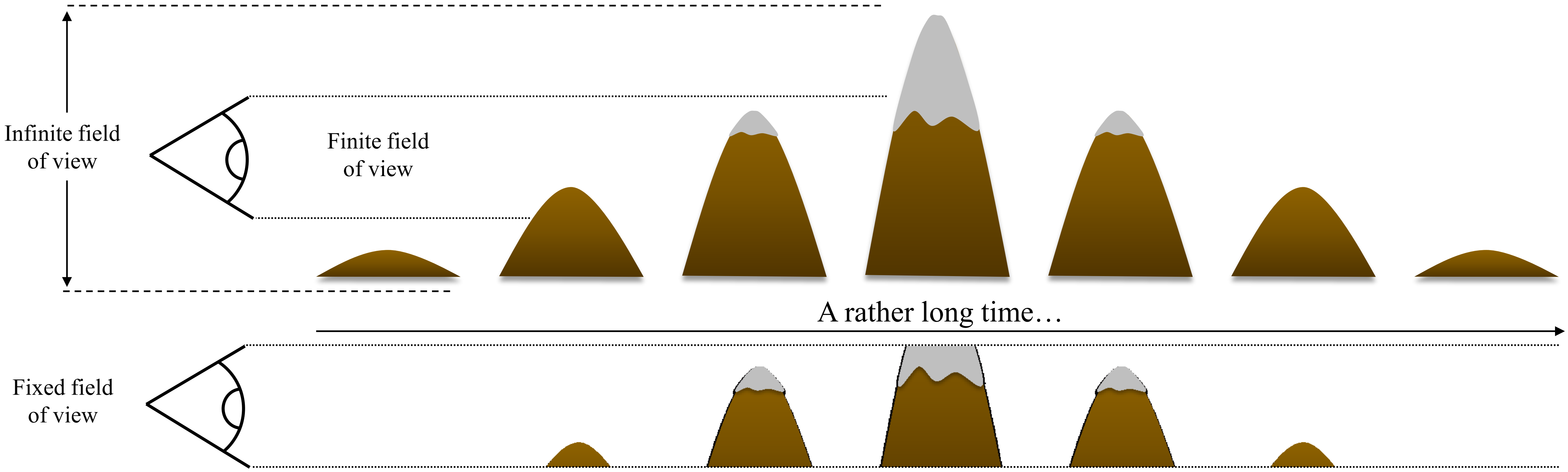


Example applications:
Investigating the role of slip systems in cold-dwell fatigue for aerospace alloys (Worsnop *et al.* (2022) *Nature Comm.*)
Control of crystallographic texture for improved formability of magnesium alloys (Roumina *et al.* (2022) *Acta Materialia*)
….

The need for dynamic range: a user perspective

To timelapse the life of a mountain…

(analogy and graphics courtesy S. Gustafson @ CHESS)

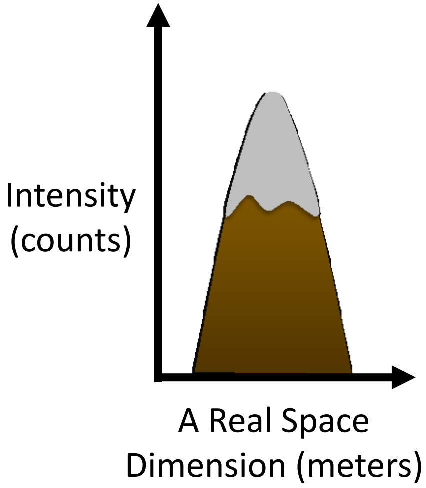


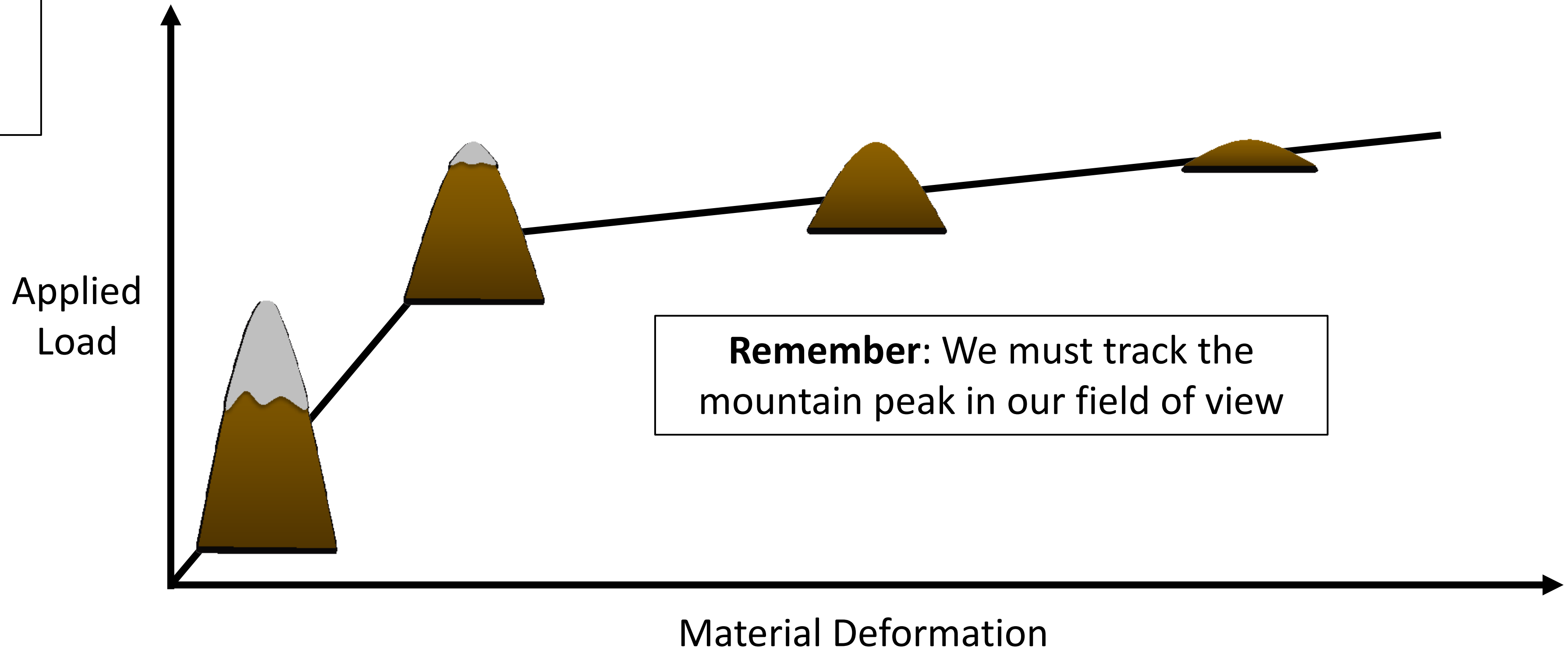
Imagine now, that the **mountain peaks are our signal**, our **detectors have limited fields of view** (dynamic range), and a full experiment can happen in minutes

Diffraction signals are moving targets

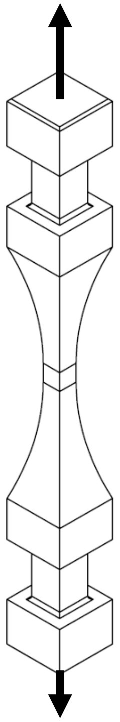
Say you go to a synchrotron and wish to do a simple metallic deformation experiment…

Our samples produce diffraction signals that resemble mountains…





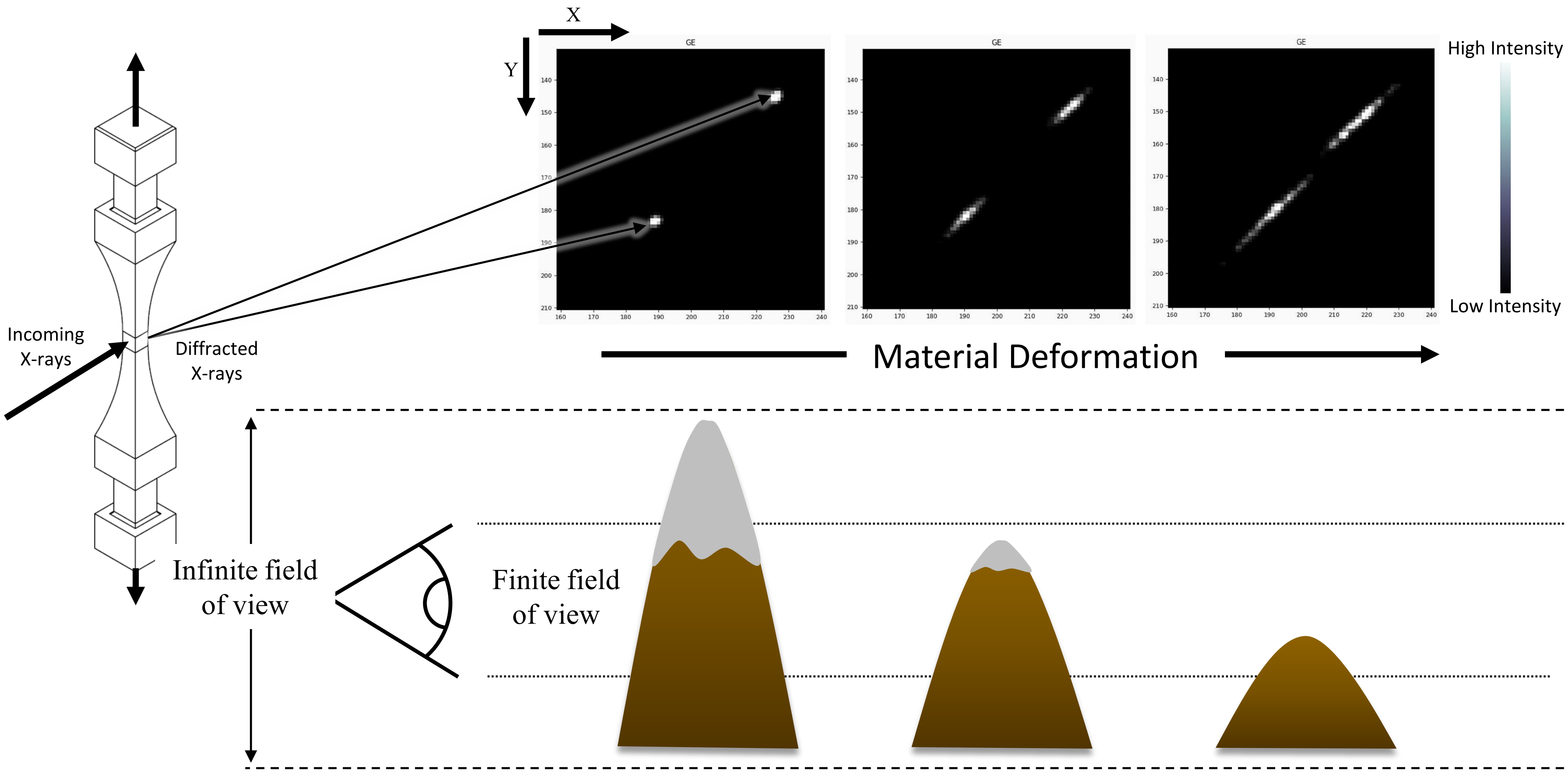
Remember: We must track the mountain peak in our field of view



Material state change -> Signal change

What changes in our signal?

Now, the same deformation experiment but with x-rays…



Peak intensity change during in-situ experiment

What changes in our signal?

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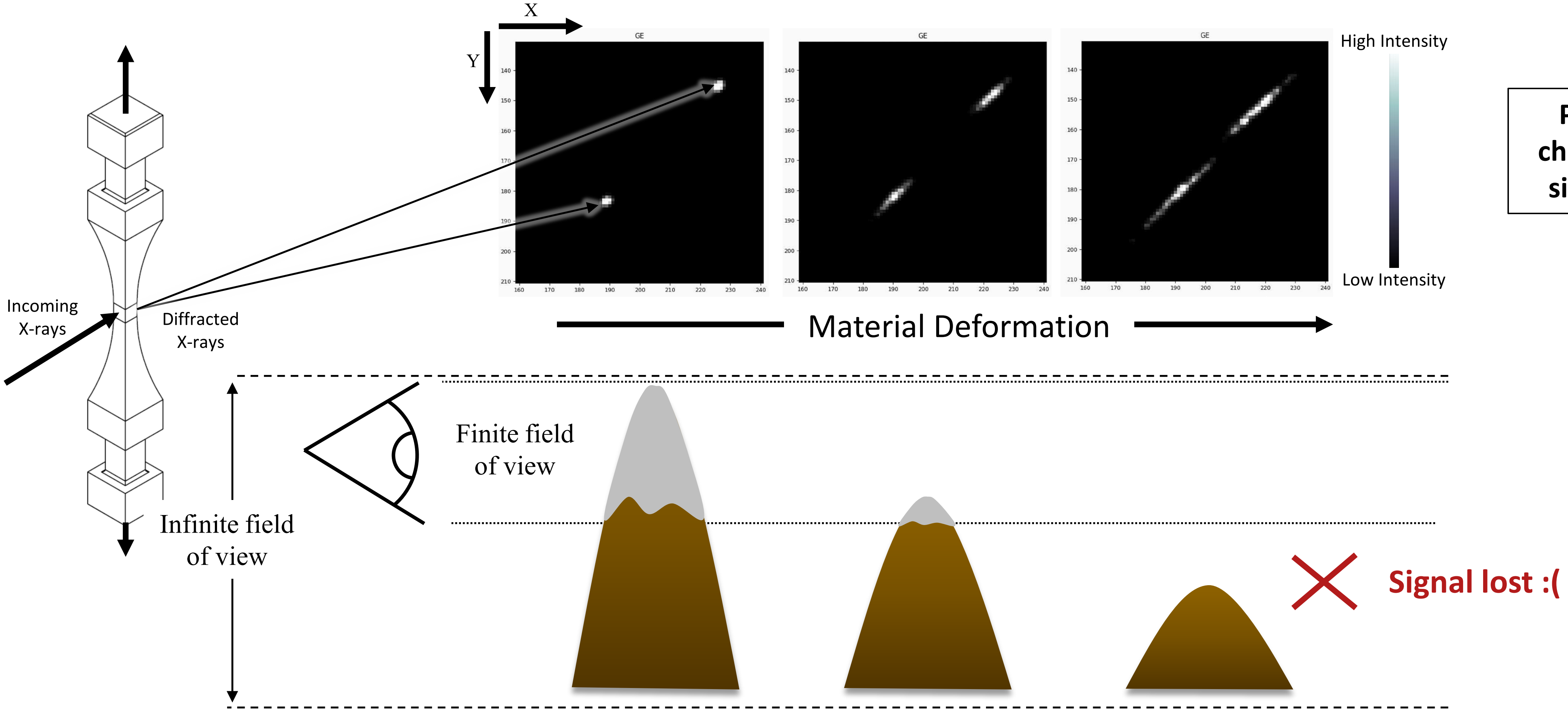


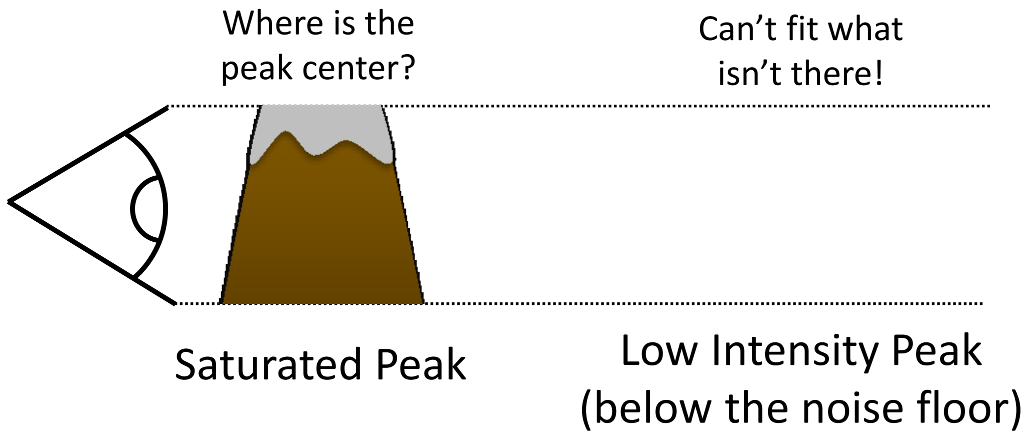
Peak intensity change during in-situ experiment

We must be able to fit our peaks

The accuracy and resolution of our techniques rely on our ability to fit centroids to each diffraction peak

Peak intensity

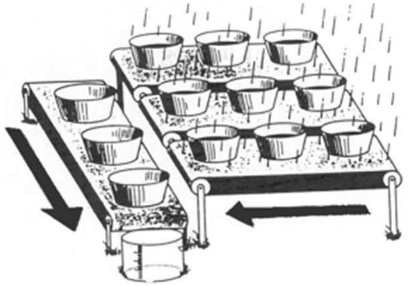
- Why do we care?
  - Peaks will either saturate, or fall below the noise floor
- Can we control it?
  - Yes! Through attenuation or exposure time



Wide-dynamic-range detectors to the rescue!

- Standard/typical detectors for 3DXRD (GE RT-41, Dexela 2923) have limited dynamic range (2-3 orders of magnitude)
- Choice driven by need for **large active area** with good stopping power in the **20-100 keV** range (at an "affordable" price…)
- Current best alternative: large area photon-counting PAD (e.g. CdTe Eiger 16M)
- BUT: we *need* photon-integrating options with comparable dynamic range to avoid systematics due to incident photon rate (see e.g. Imai & Hatsui JSR 2024)

Challenge: extending the dynamic range of integrating detectors



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Counting
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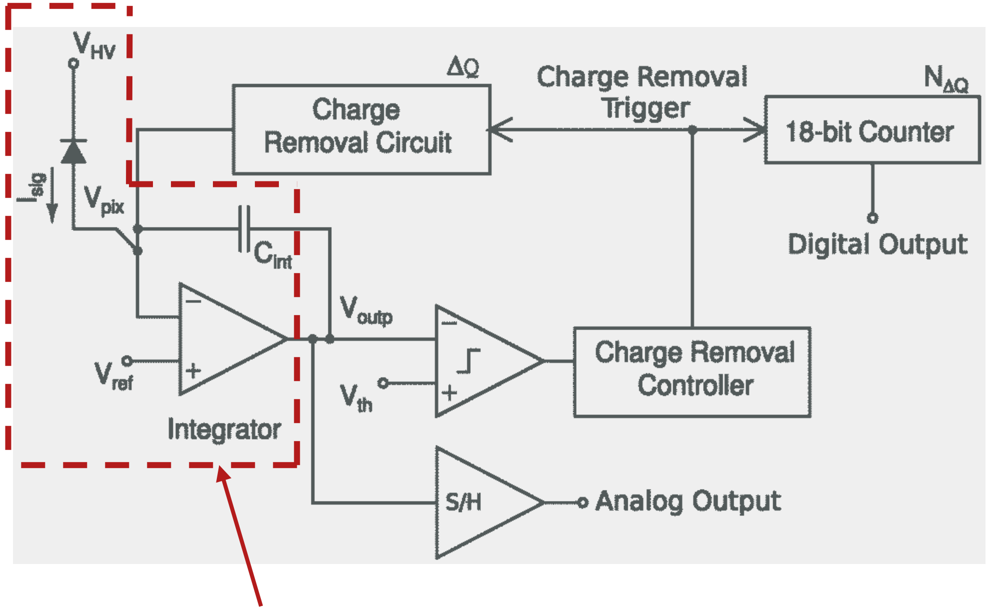
- Photon rate limit ~10^6 ph/pix/s

How do we keep the rate-limit benefits of an integrating detector, but extend the dynamic range to something like that of a counting detector?

Mixed-Mode PAD (MM-PAD)



In a purely integrating pixel: well depth limited by feedback capacitance C_{int}

- Voltage swing typically ~1 V, feedback capacitance up to 2 fF/µm^2 → **~1.2x10^5 8-keV ph/pix** max in 150 x 150 µm pixel

Charge removal decouples well depth from C_{int} to provide extended dynamic range

Specification	MM-PAD-1.0* (8 keV equivalent)	MM-PAD-2.1† (20 keV equivalent)
Status	Medium-scale lab prototypes operational; commercial units in progress	Pixel design fully vetted; medium-scale lab prototypes in progress
# of pixels per chip	128 x 128	
Pixel size	150 µm	
Frame rate	1.1 kHz	≥1.1 kHz
Duty cycle at max FR	~0%	≥ 90%
Read noise	0.16 photon	0.13 photon
Well capacity	4.7x10^7 photons	2.2x10^7 photons
Instantaneous photon rate	> 10^{12} ph/s/pix	> 10^{12} ph/s/pix
Sustained photon rate	4x10^8 ph/s/pix	3x10^{10} ph/s/pix

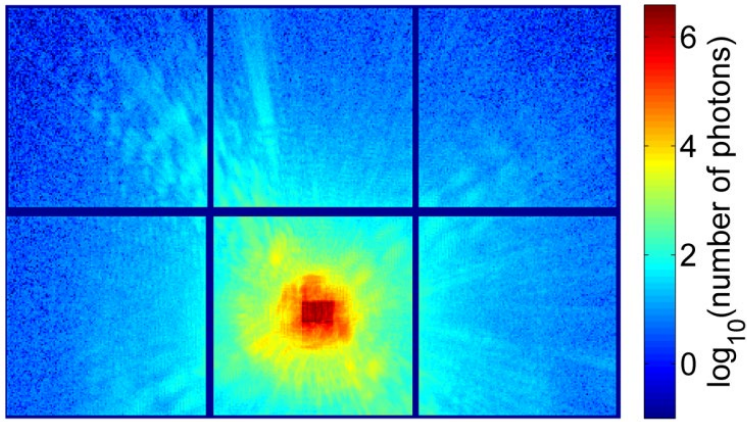
*Tate *et al.*, *Journal of Physics: Conference Series* (2013)
†Gadkari *et al.*, *JINST* (2022)

MM-PAD: applications

Wide dynamic range gives **extraordinary experimental flexibility**

Coherent diffractive imaging

PETRA-III / Mancuso (Eu-XFEL)

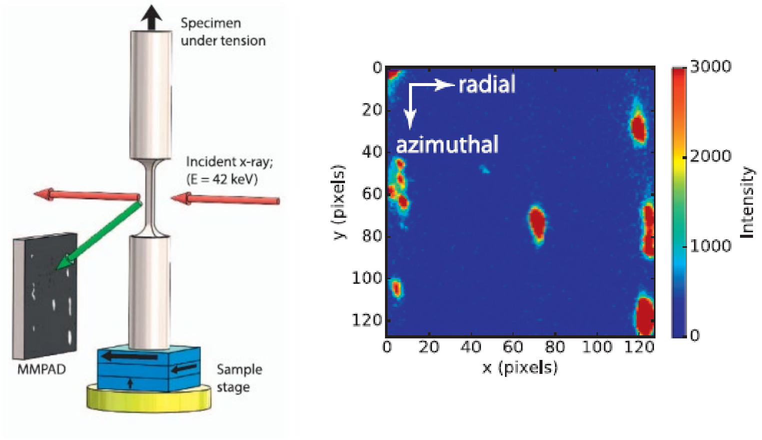


Giewekemeyer et al., *Journal of Synchrotron Radiation* (2014)

- Capture scattering pattern from Au test object, allowing ptychographic image reconstruction with ~25nm resolution
- **Key detector features:** wide dynamic range, fidelity at high incident photon rates (**>10^7 ph/pix/s** in central spot)

Deformation in metals

CHESS / Beaudoin (U. Illinois)

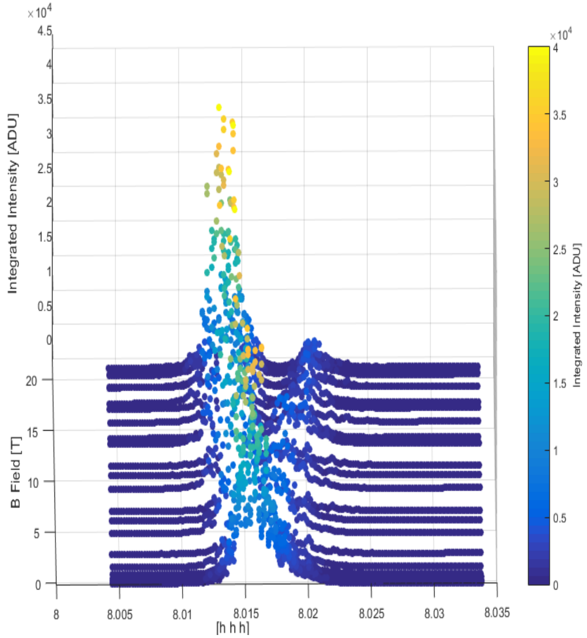


Chatterjee et al., *J. Mechanics & Physics of Solids* (2017)

- Probe grain-level deformation mechanisms and residual stress in polycrystalline Ti-7Al alloy under applied stress gradient
- **Key detector features:** CdTe sensor for efficient detection of 42 keV photons

Piezomagnetic ordering in UO2

APS / Gofryk (Idaho Nat'l Lab)



Antonio et al., *Nat. Communications Materials* (2021)

- Observe Bragg peak splitting in UO2 during 10ms magnetic pulse
- **Key detector features:** Fast (1 kHz) continuous frame rate

MM-PAD-2.1 pixel

improvements to MM-PAD pixel

Developed in TSMC 180nm process via 4 MPW submissions over 2014-2018

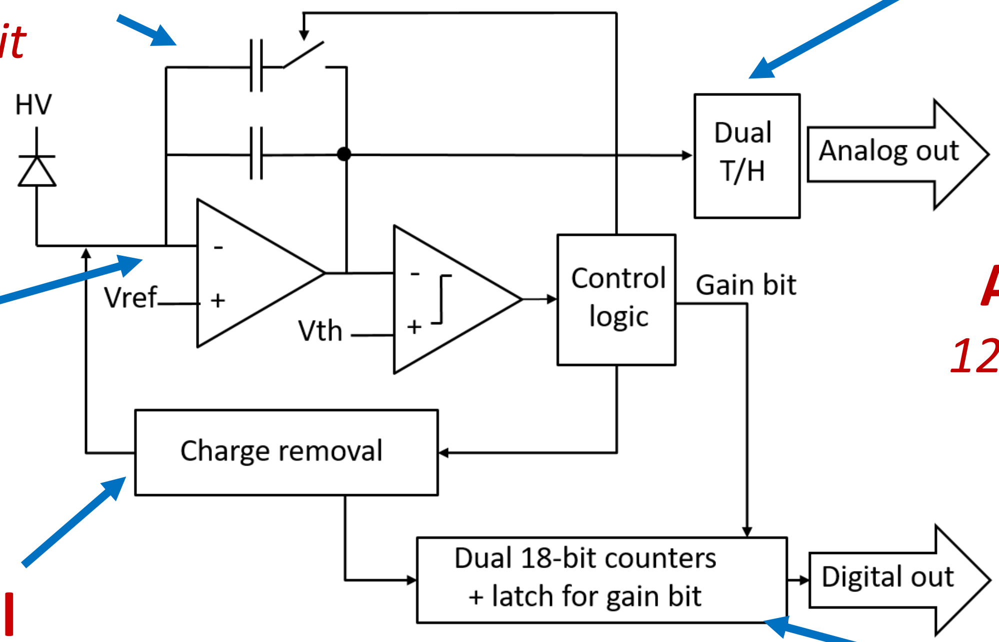
Adaptive gain

Maintain high SNR at low signal levels while larger low-gain cap increases sustained flux limit

Dual track/hold circuit

Differential output

Expose-during-readout operation



Class AB amplifier

higher slew rate

Faster readout:

ASIC capable of < 100 ns/pixel

128 x 128 pixels in 16 channels: ~10 kHz

8 channels: ~5 kHz

4 channels: ~1 kHz

Faster charge removal

100 MHz max operation

Dual in-pixel counters

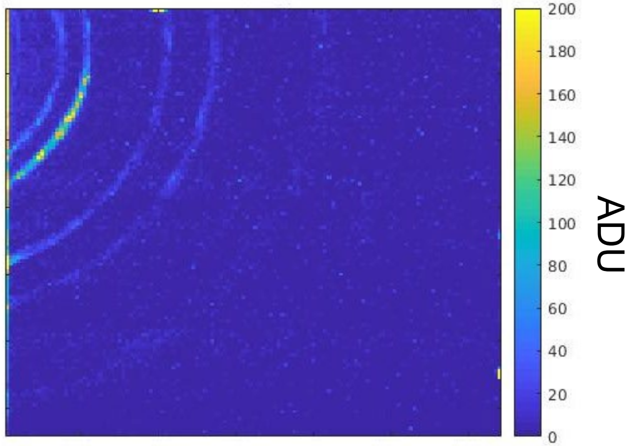
Expose-during-readout operation

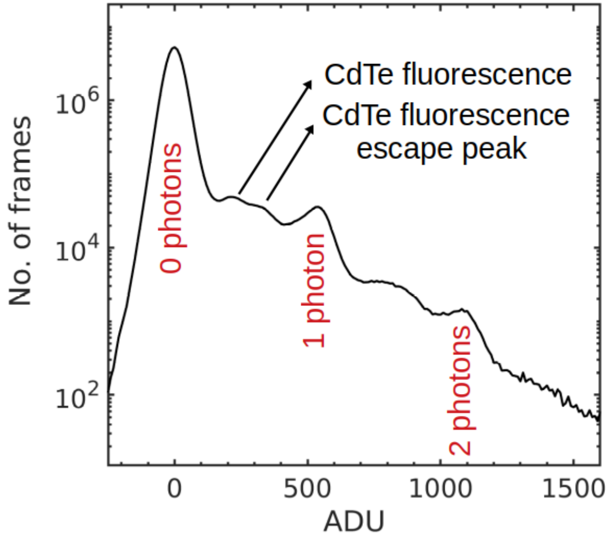
Full system: collaboration with detector group at APS | APS: firmware, support electronics | Cornell: ASIC, sensor

Full-scale ASIC characterization

- 128x128 pixel full-scale ASIC fabricated in early 2020
  - May 2021: tests with CdTe single-chip modules at CHESS FAST/ID3A – 61 keV photon energy

Low-flux characterization

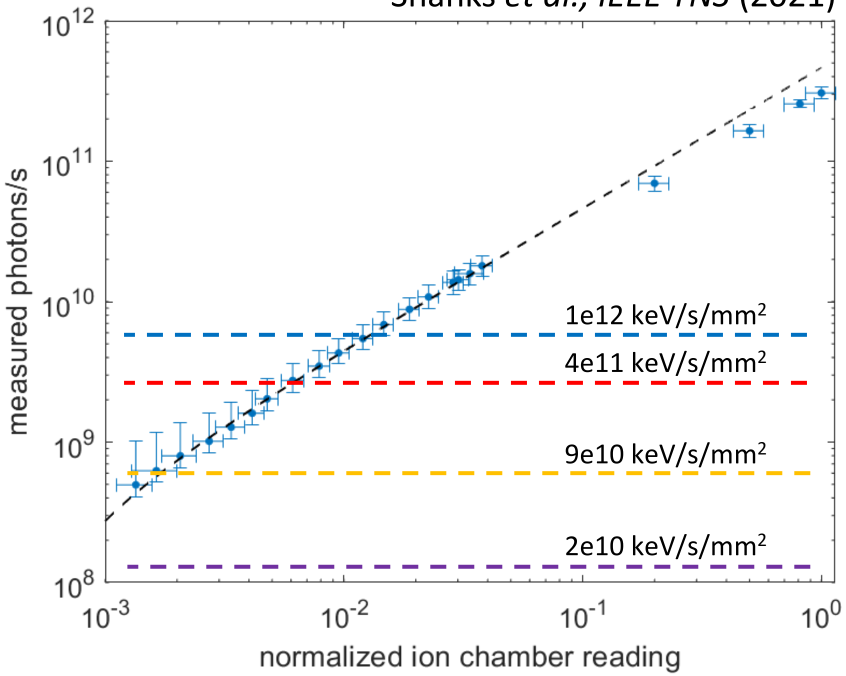




High-flux characterization

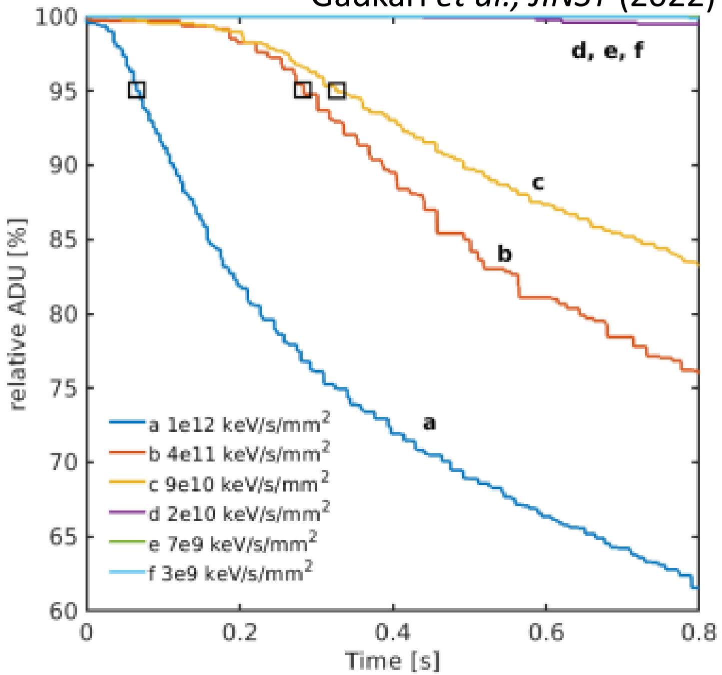
Pixel performance (small-scale chip) with Si sensor, 10 keV x-rays (APS 6-ID-C)

Shanks *et al.*, *IEEE TNS* (2021)



Pixel performance (full-scale chip) with CdTe sensor, 61 keV x-rays (CHESS ID3A)

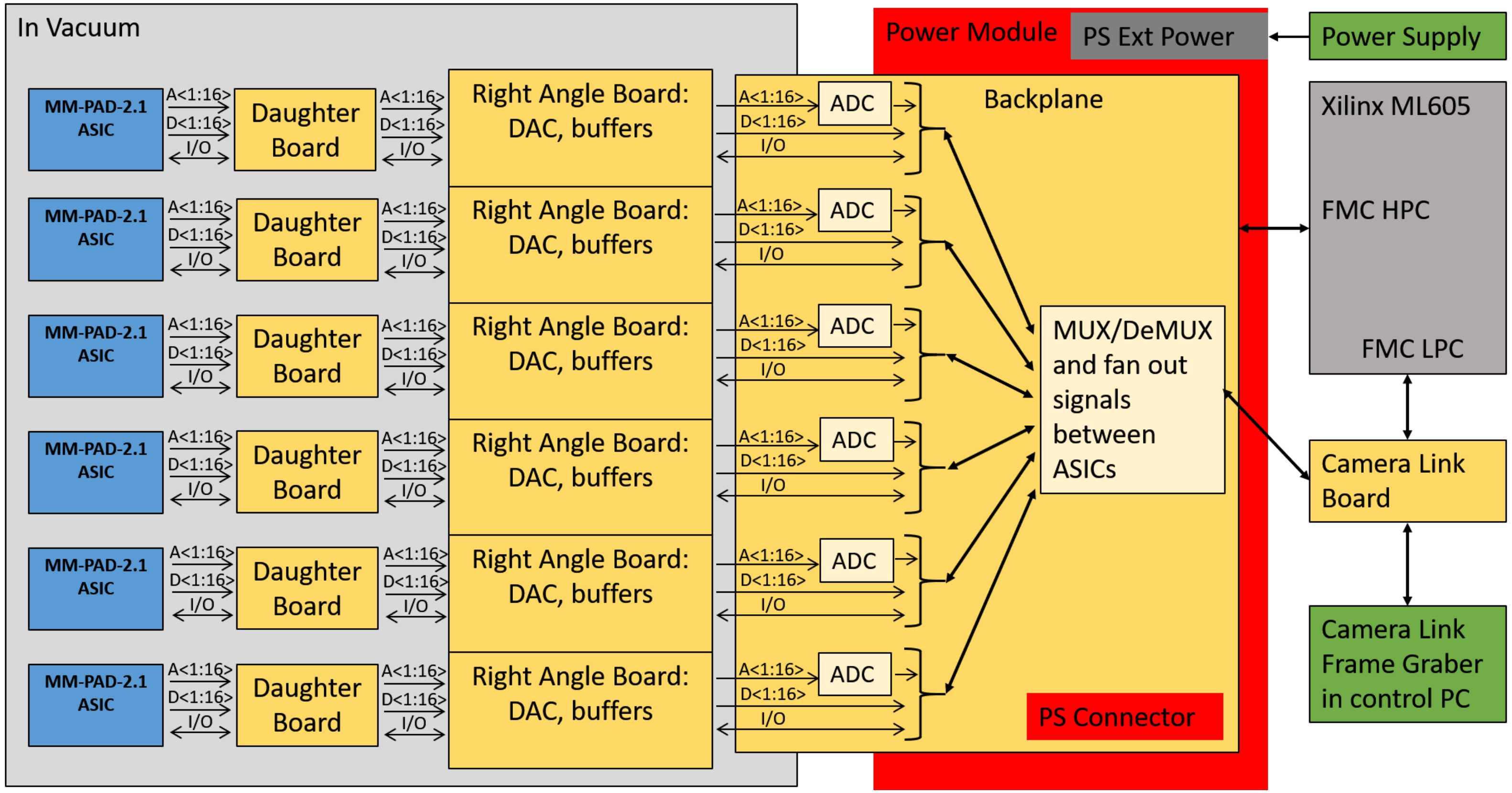
Gadkari *et al.*, *JINST* (2022)



CdTe polarization observed well before ASIC becomes photon-rate limited
→ Acute need for alternative high-Z sensors
→ Ongoing investigations into aSe, CZT, Ge (with APS, BNL, SLAC; MIT-LL)

Readout system and project status

Readout system block diagram for 6-module MM-PAD-2.1



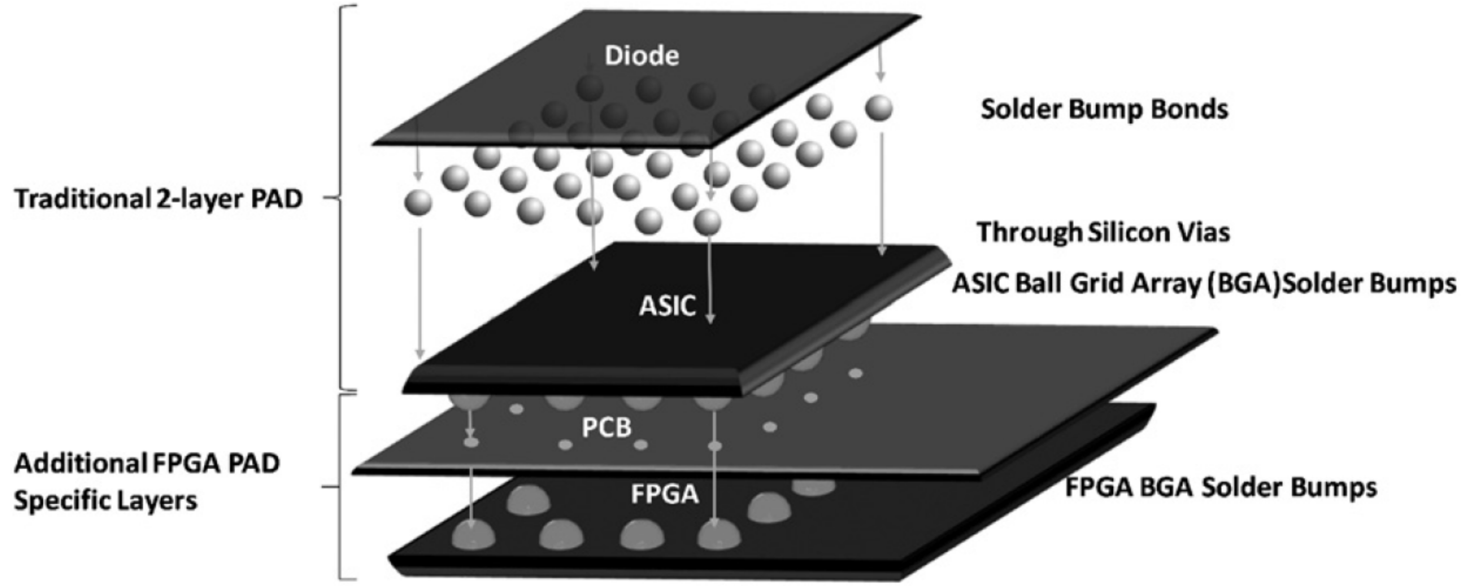
Project status

- Single-chip Si, CdTe hybrids have been assembled
- May 2021: high-flux testing at CHESS using single-chip readout system adapted from EM-PAD-II (MM-PAD variant for STEM)
- Test/debug of full-system readout electronics currently ongoing
- Selectable readout of full array at continuous frame rate of **1.6 kHz** or 128x128 pixel area at **9 kHz**

The data rate problem

Wide dynamic range + high frame rate + lots of pixels = too much data, too fast…
How do we solve the data rate problem AT the detector?

One concept: leverage *detector firmware* to deploy flexible, field-programmable data compression/reduction/monitoring tools *in-line*, before any data is saved



Hromalik (2013) *NIMA*

Problems:

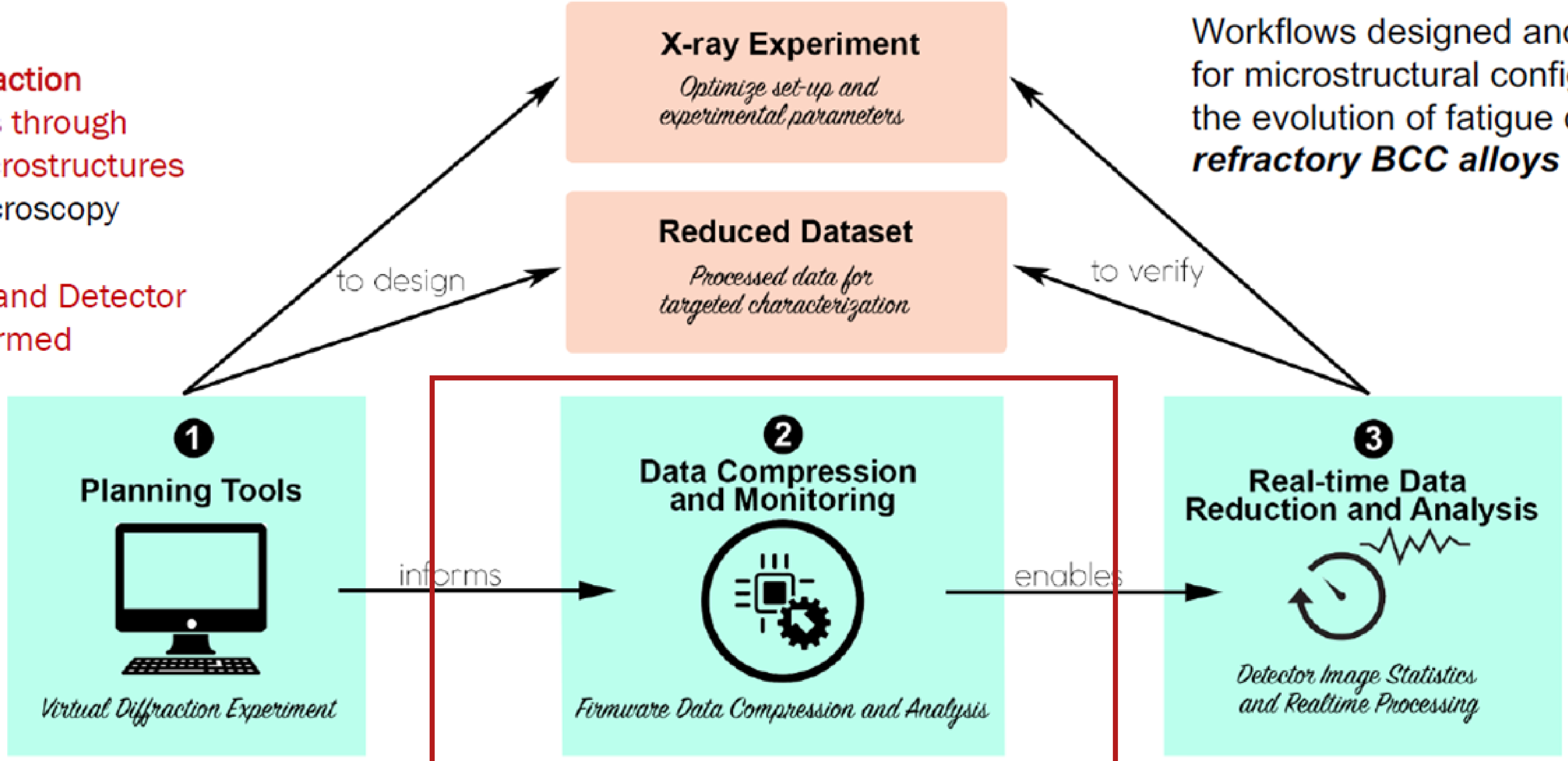
- this physical integration is high-risk and expensive
- *Not* saving full-frame raw data feels risky – *are we sure we know what signals we care about?*

Data-intensive science requires coordinated tools

- Virtual Diffraction experiments through meshed microstructures
- Electron Microscopy informed
- Instrument and Detector Physics informed

Workflows designed and demonstrated for microstructural configurations and the evolution of fatigue damage in ***refractory BCC alloys***

User Facing



User Facing

- Only collect data you need
- Know what SIGNALS are relevant
- Leverage other modalities

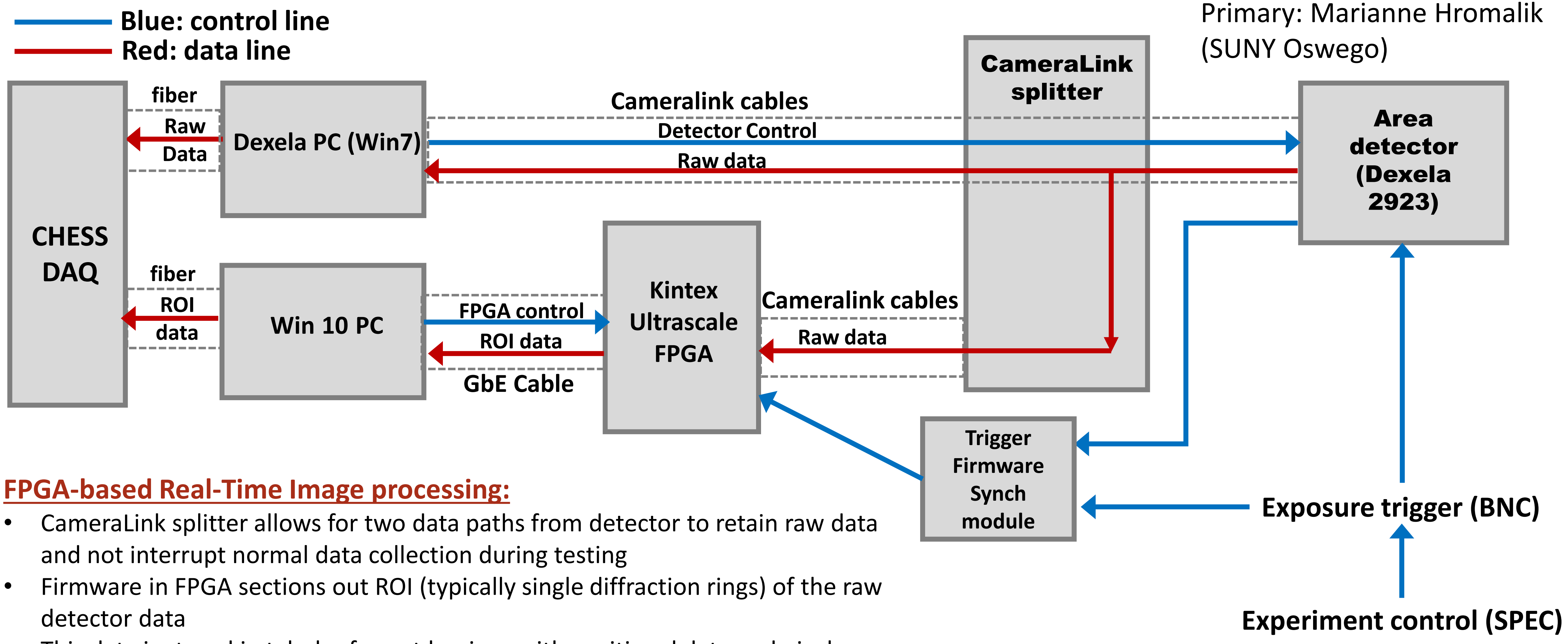
- Inline Firmware data compression and monitoring using FPGA
- Lossless and lossy methods
- Trust these decisions through planning

- Use planning tools and create proxies for on-the-fly analysis

Team: CHESS, UCSB, Tufts, SUNY Oswego

A setup for FPGA-based real-time image processing

Primary: Marianne Hromalik
(SUNY Oswego)



FPGA-based Real-Time Image processing:

- CameraLink splitter allows for two data paths from detector to retain raw data and not interrupt normal data collection during testing
- Firmware in FPGA sections out ROI (typically single diffraction rings) of the raw detector data
- This data is stored in tabular format by rings with positional data and pixel values for pixels.
- This reduces the data to be processed to be used by signal processing software.
- Timestamp FPGA data with Trigger signal to synchronize to raw data frames.

Summary

Wide-dynamic-range area detectors are critically needed at synchrotron beamlines in order to advance diffraction-based techniques – especially for dynamic studies.

High-energy diffraction microscopy (aka 3DXRD) is a prime example of an application requiring increased dynamic range.

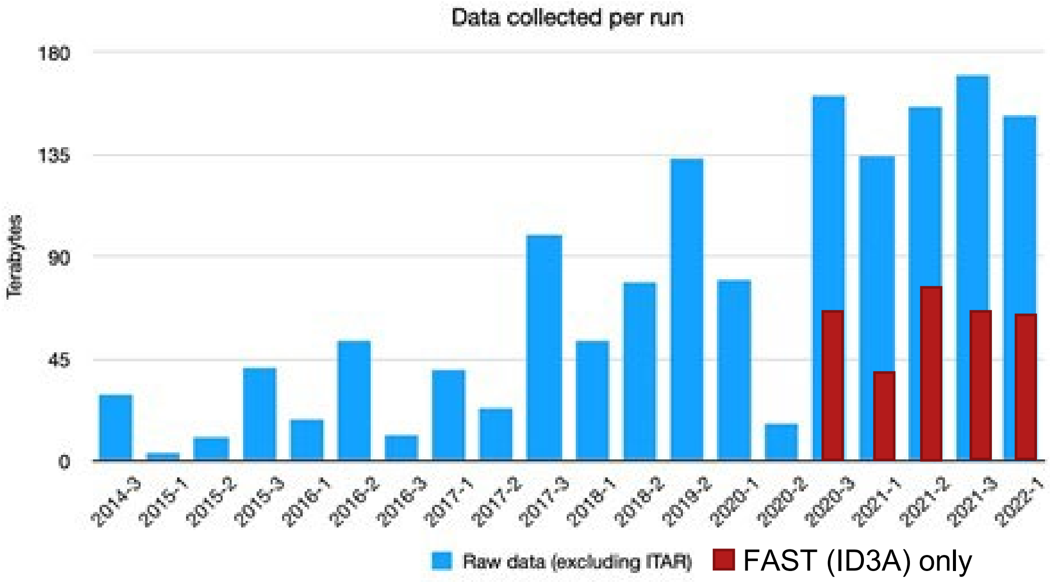
The **MM-PAD family** of detectors fills a unique “middle ground” combining key benefits of photon-integrating and photon-counting architectures.

Increases to dynamic range + frame rate must be accompanied by new strategies for managing **large data volumes** and **high data rates**.

Thank you!

Backup slides

Postscript: The Data Problem



Since the facility upgrade in 2019, researchers at CHESS have collected **1.0 PB of raw data** across 7 beamlines

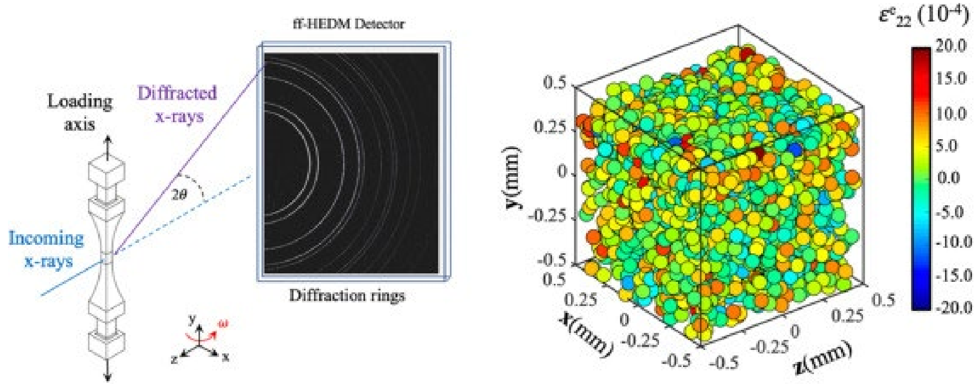
Data volumes are an issue both after beamtime…
- Storage challenges (disk space, file transfer, data preservation)
- Computing challenges (software, efficiency, speed)

… and also **during** beamtime:
- Challenges extracting information from or visualizing large datasets -> difficult for users (especially novices) to make informed decisions on-the-fly about data collection strategy

Detector strategies: in-line sparsification, compression, event-driven readout + triggering

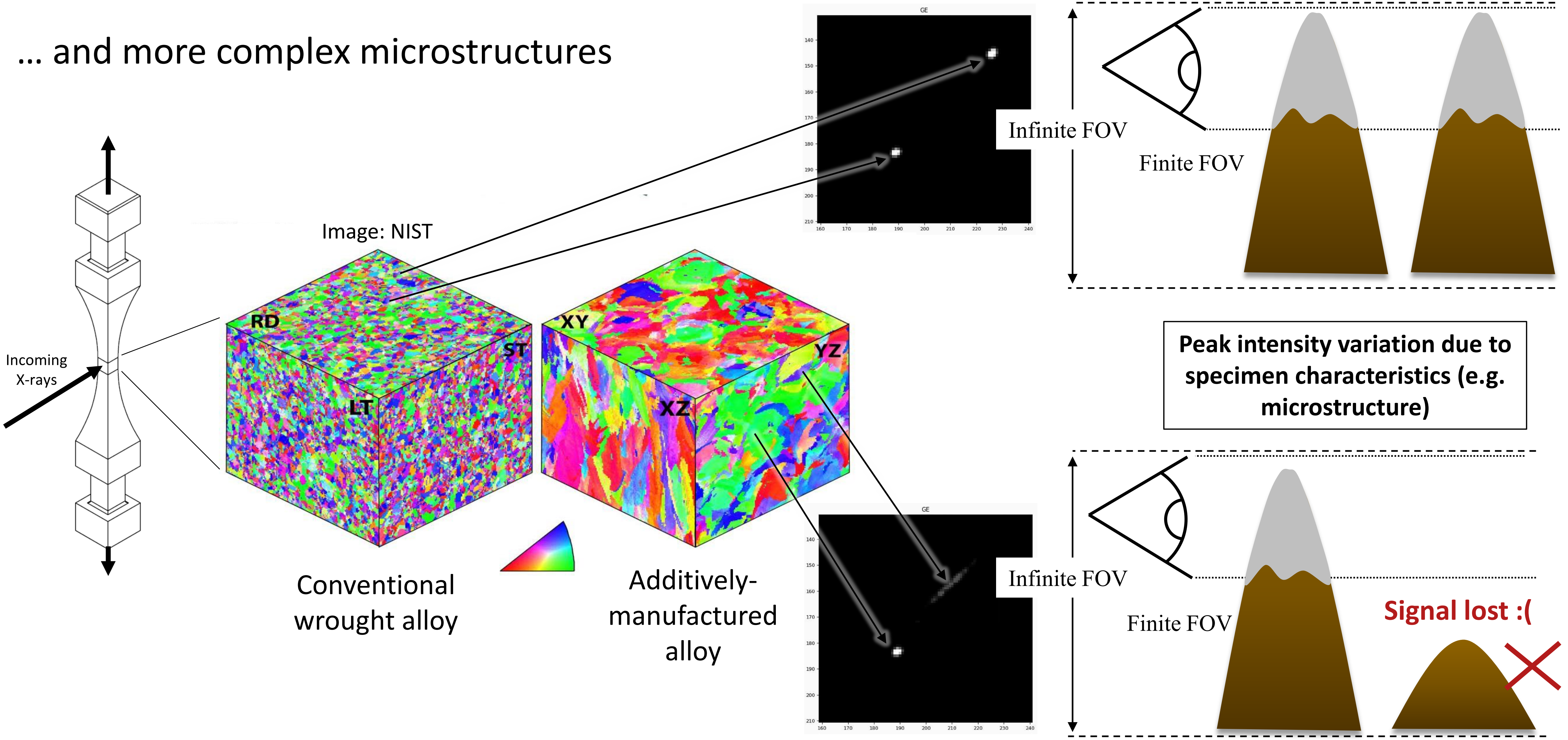
Proposed broader approach: interface these detector-side strategies with *domain-science-informed experiment planning tools* (e.g. simulation, virtual diffractometer) to build user confidence, ensure data integrity, and achieve better scientific outcomes

<u>Use case: high-energy diffraction microscopy (HEDM)</u>



What changes in our signal?

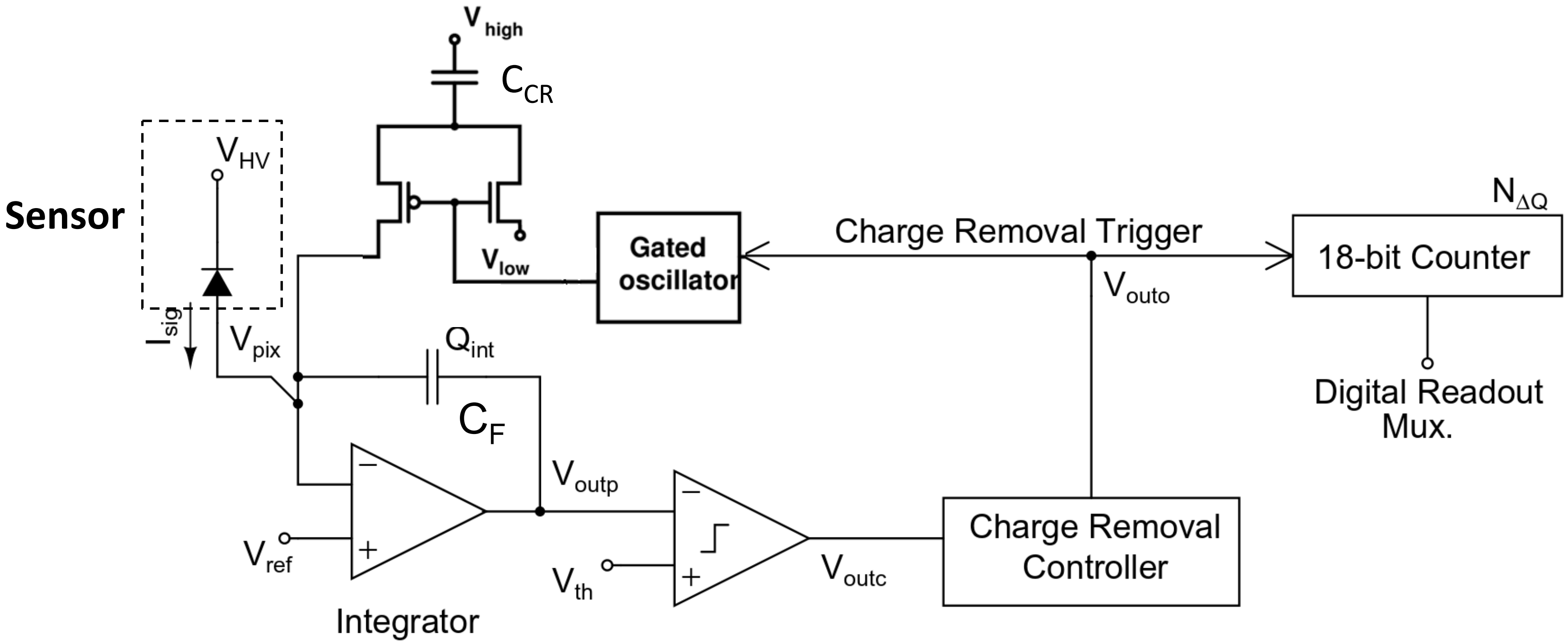
... and more complex microstructures



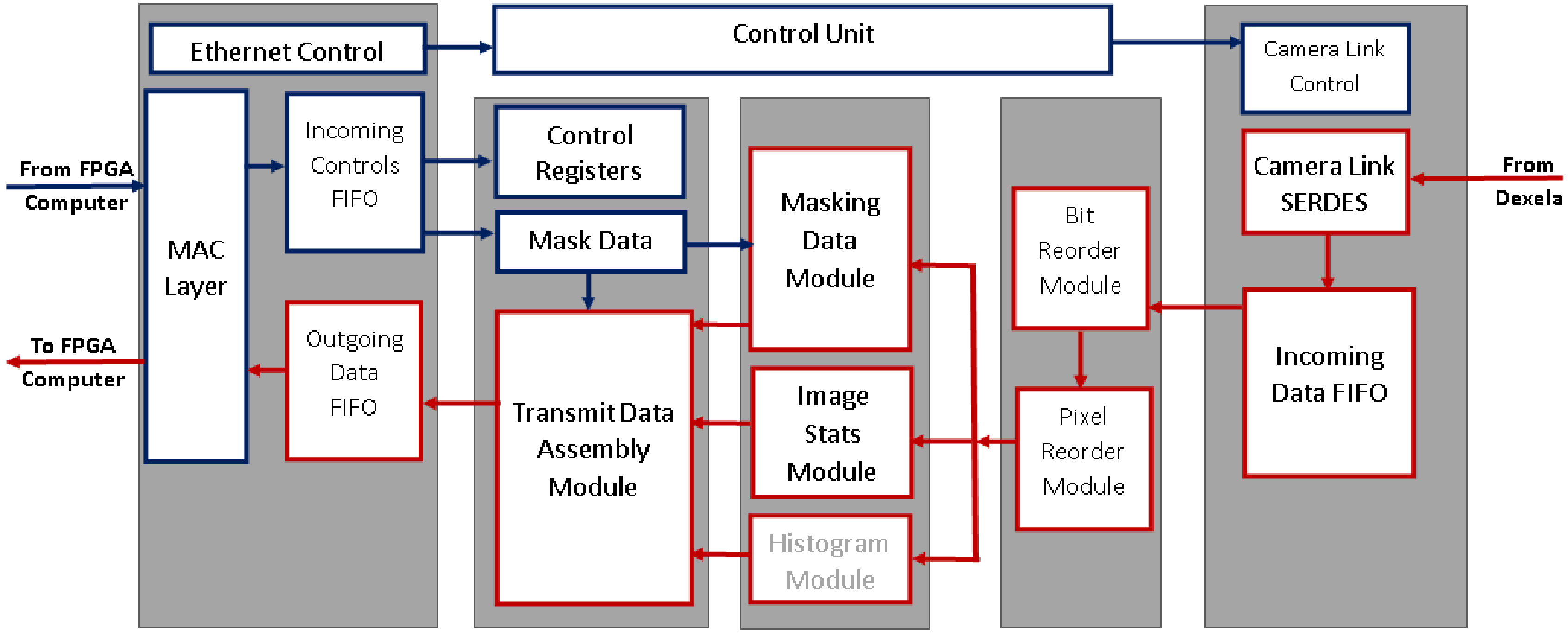
First-generation MM-PAD: Limitations

- **Readout limited to ~0% duty cycle at max frame rate of 1.1 kHz**

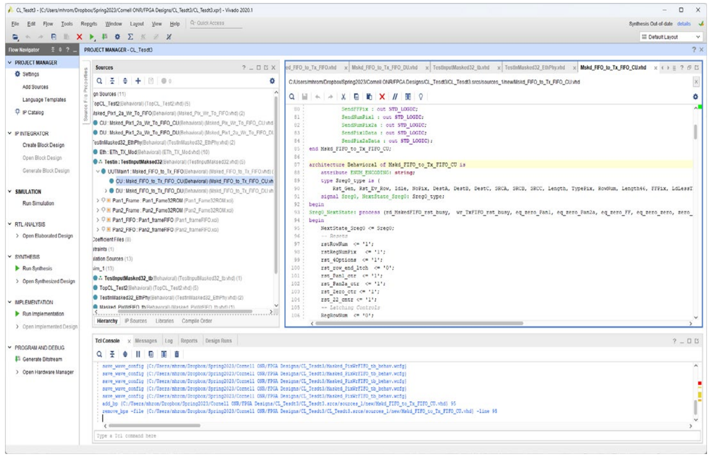
- **Charge removal circuitry runs at 2 Mhz max**
  - 4×10^8 8 keV x-rays/pix/s max sustained photon rate



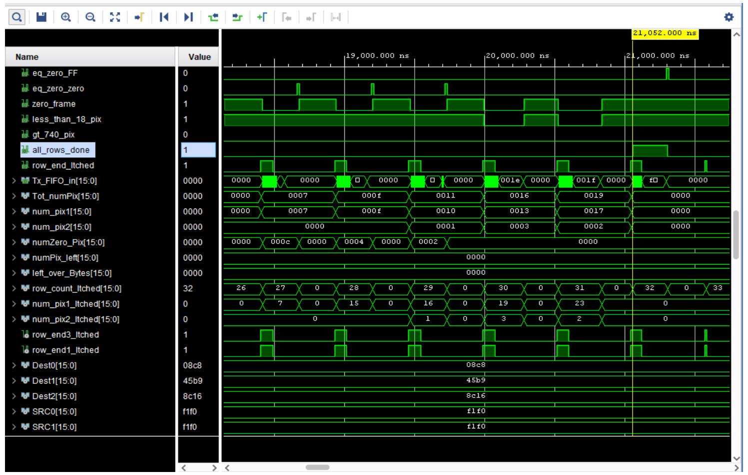
Firmware data acquisition, processing and control



Firmware Modules implemented within the Kintex UltraScale XCKU040 FPGA



Modules were designed in VHDL in Vivado IDE



Modules were individually and collectively simulated in Vivado Simulator

Within the FPGA:

- Dexela CameraLink data was fed into the XCKU040 FPGA on the KCU105 board:
  - Deserialized, buffered and re-ordered
  - Masked using the stored ROI information
  - Buffered and transmitted via GbE to the FPGA Computer
- All modules were designed in VHDL using Xilinx/AMD Vivado IDE
- All modules were individually and then collectively simulated using Vivado Simulator
- Real-time signal acquisition for trigger testing was achieved using Vivado ILA (Integrated Logic Analyzer)