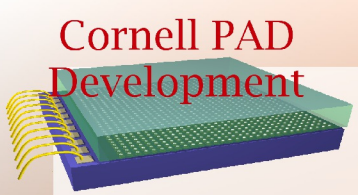
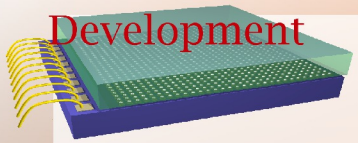


Low-information frames, random orientation, real detectors, real data.

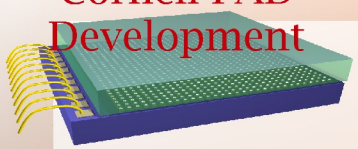
Hugh Philipp
htp2@cornell.edu
Kartik Ayyer, Mark Tate, Veit Elser, Sol Gruner

SRI 2012
July 2012
Lyon, France

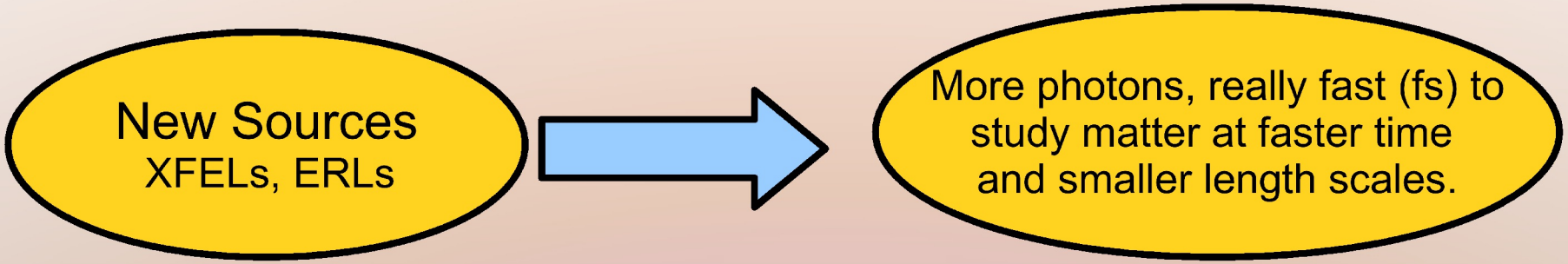


Introduction

- Talk about two things:
  - Dealing with low-fluence data from integrating detectors.
  - Using this data in the context of randomly oriented sample, low-information snap-shots.



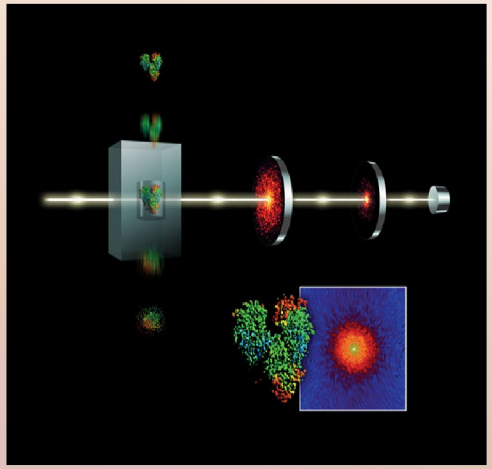
Data Data Data



- Small things (atomic scale)
- Time scales small (fs)
- Difficult to control orientations
- Small things scatter less (fewer photons)
- Exploiting fast resolution → dealing with data of particular type

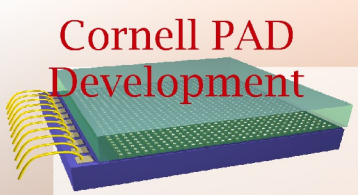
Data Data Data

New Sources
XFELs, ERLs



- Small things (atomic scale)
- Time scales small (fs)
- Difficult to control orientations
- Small things scatter less (fewer photons)
- Exploiting fast resolution → dealing with data of particular type.

Low fluence data, of the randomly oriented.

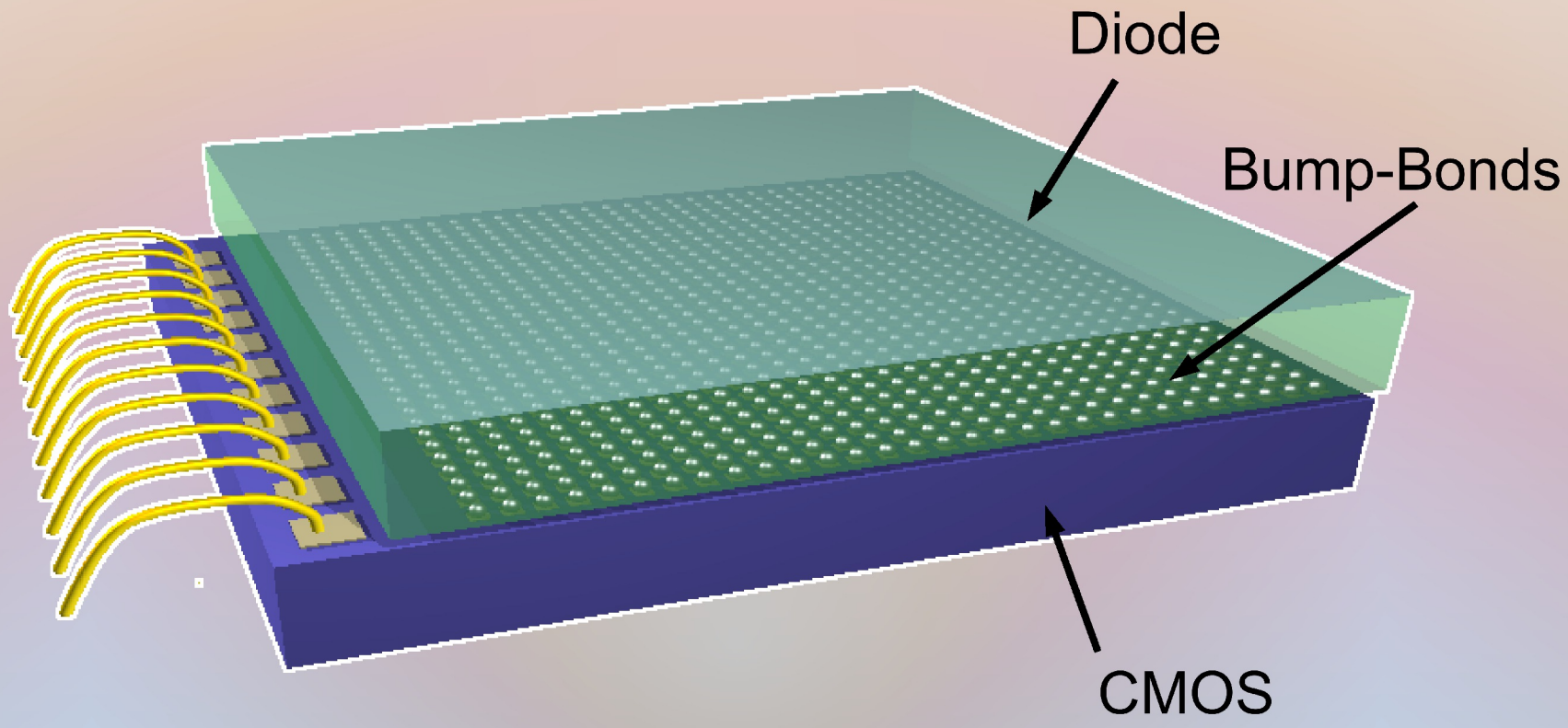


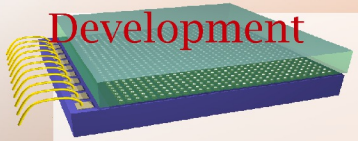
Need detectors: Requirements

- Ability to detect single photons
  - need good signal to noise.
- Able to collect data in high-fluence regions
  - can't photon count.
- Need fast frame rate (e.g. LCLS :120 Hz, European XFEL: much faster)
- Good efficiency

Pixel Array Detectors

- Direct detection in Si, good signal to noise.





Pixel Array Detectors

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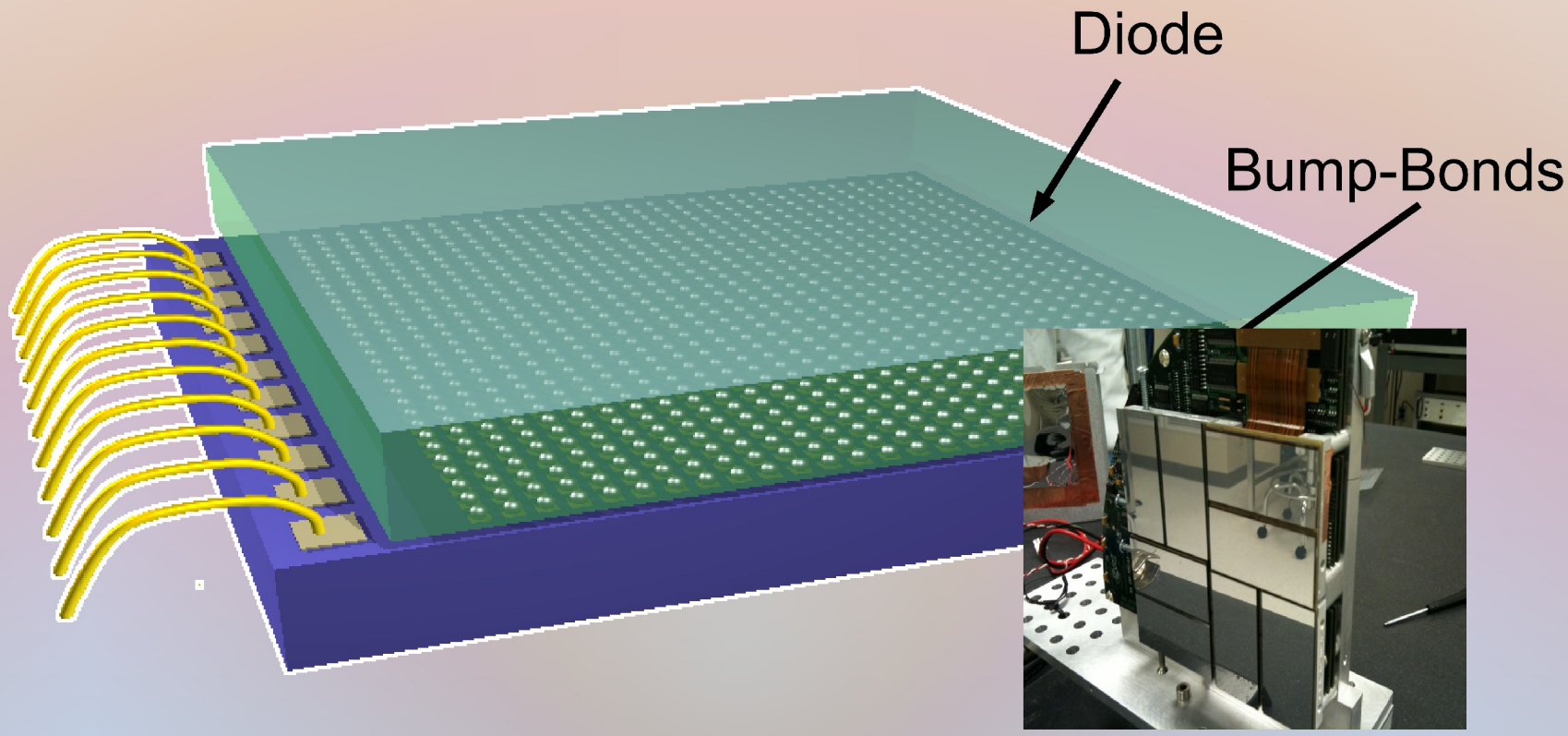
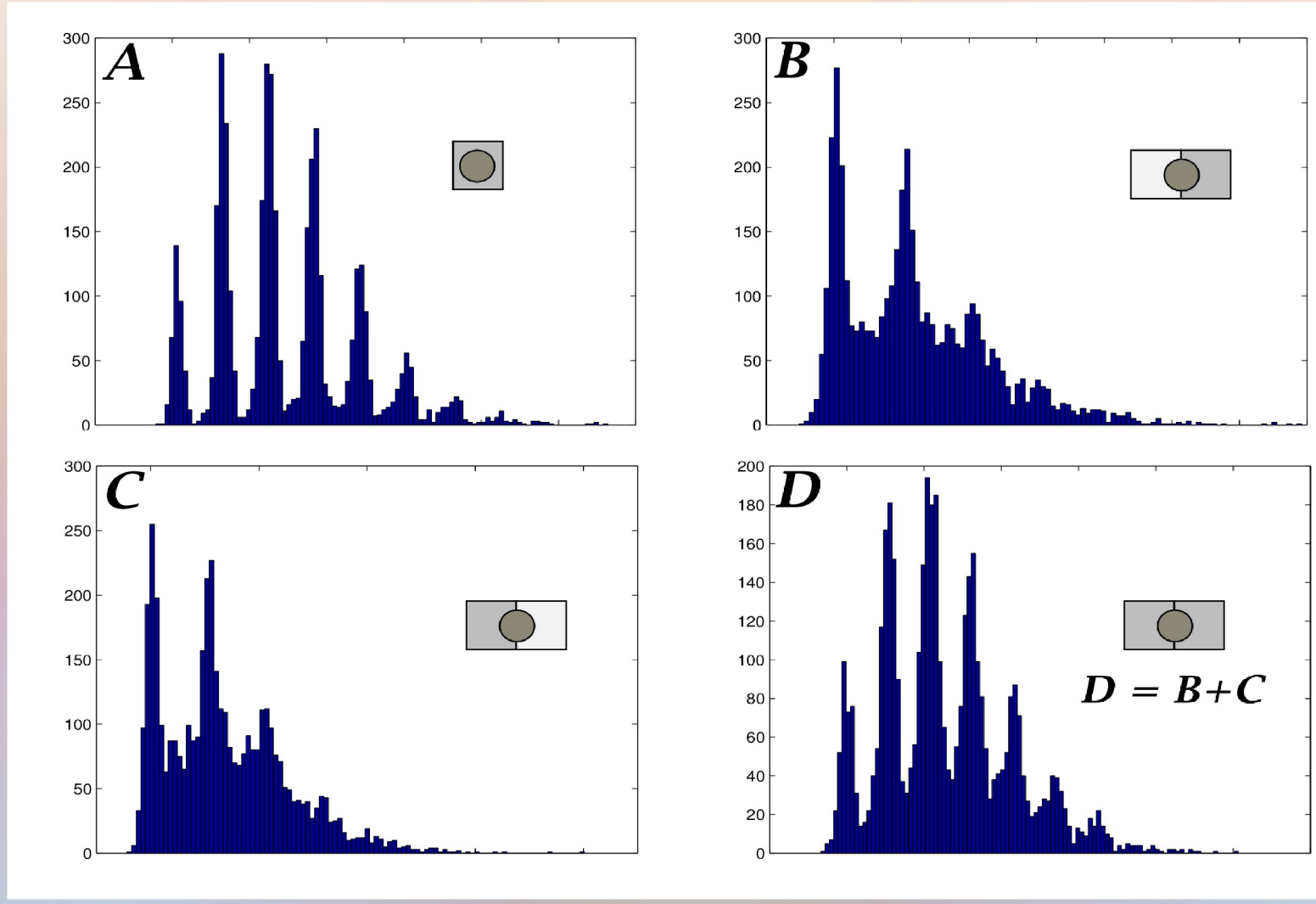


Cornell PAD Development

Single photons, integrating detector

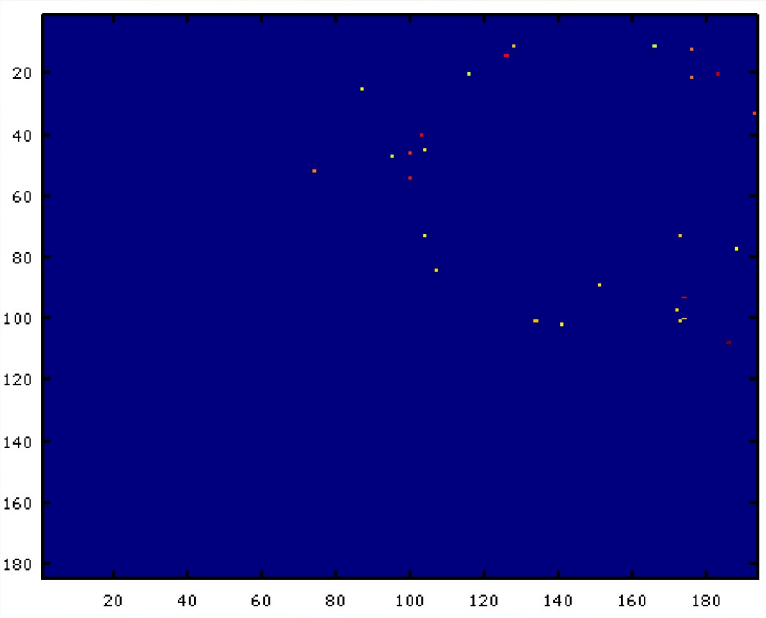


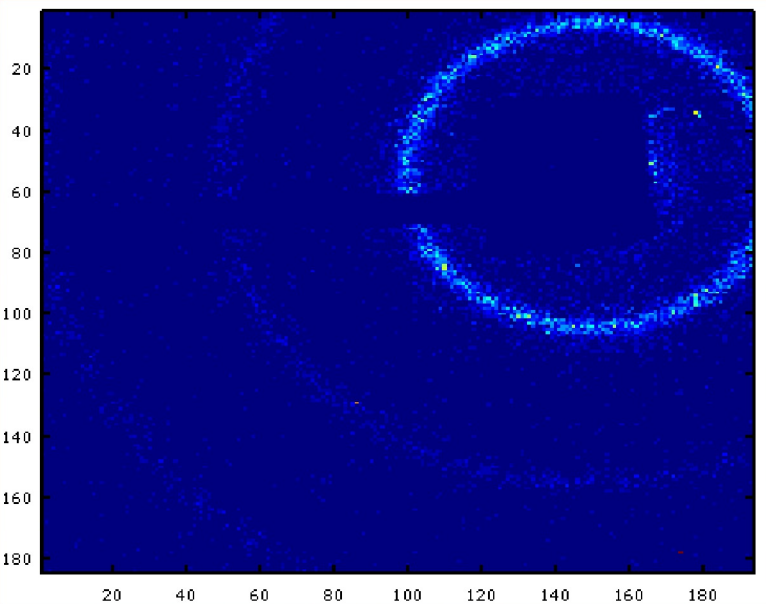
H. T. Philipp, L. J. Koerner, M. S. Hromalik, M. W. Tate, and S. M. Gruner, "Femtosecond radiation experiment detector for x-ray free-electron laser (XFEL) coherent x-ray imaging," IEEE Trans. Nucl. Sci. 57, 3795–3799 (2010).

Data taken with PAD designed for LCLS.

Cornell PAD Development

Low-fluence data





Single Frames

Added, thresholded frames
Up to ~350 frames

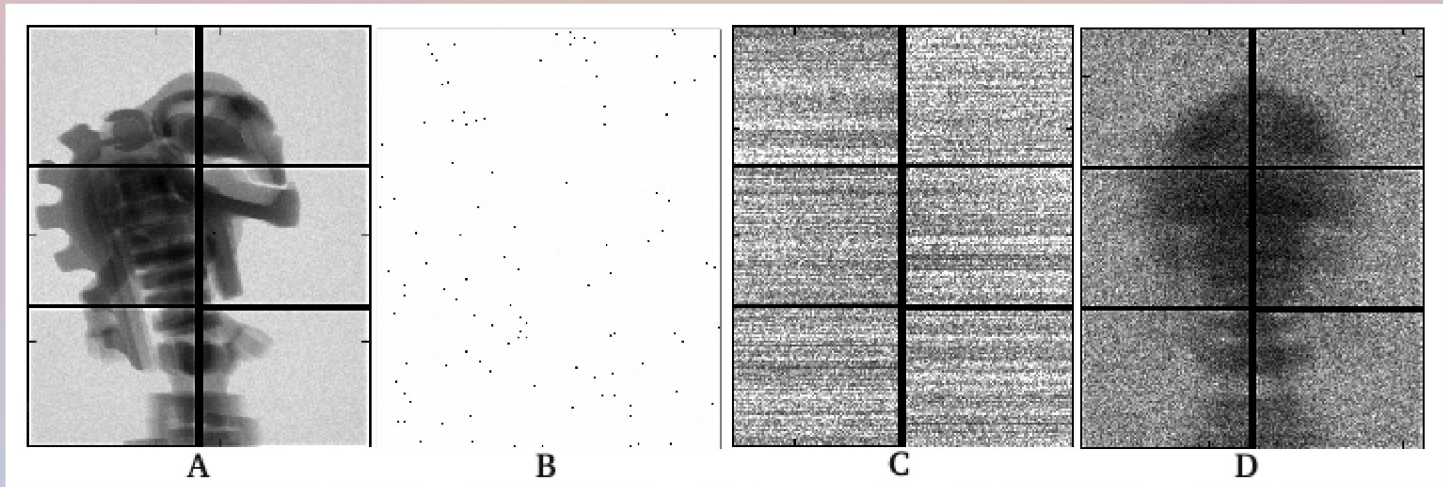
H. T. Philipp, L. J. Koerner, M. S. Hromalik, M. W. Tate, and S. M. Gruner, “Femtosecond radiation experiment detector for x-ray free-electron laser (XFEL) coherent x-ray imaging,” IEEE Trans. Nucl. Sci. 57, 3795–3799 (2010).

Data taken with PAD designed for LCLS.

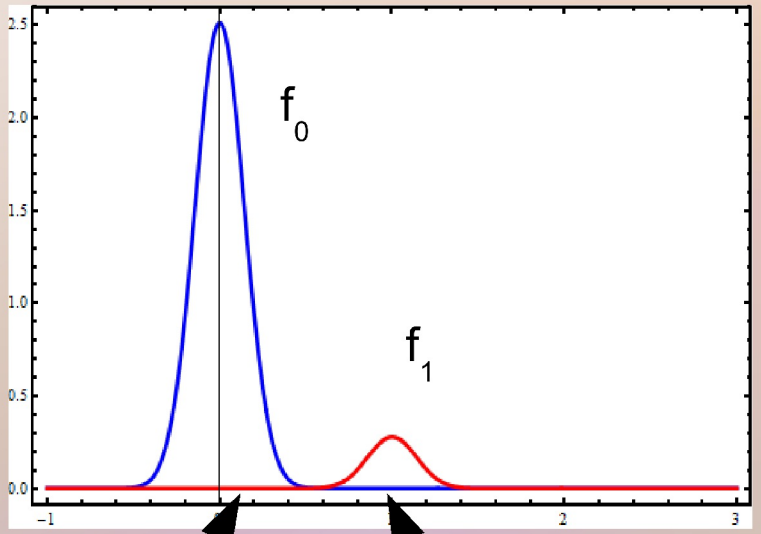
Zero level measurement

- The reference level for no signal in integrating detector is a measurement itself.
- Errors greater than average signal level →

  can't average raw frames.



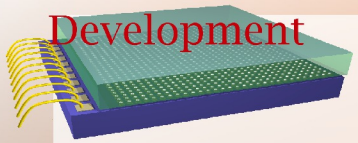
Thresholding



- Two distributions: 0 and 1 photons.
- If frequency (photon/pixel/frame) for 1 photon is A.
- Question – for an A, at what level does the threshold need f_0 'noise' is low compared to f_1 'signal'.

$$\int_{thr}^{\infty} f_0 = \int_{thr}^{\infty} f_1$$

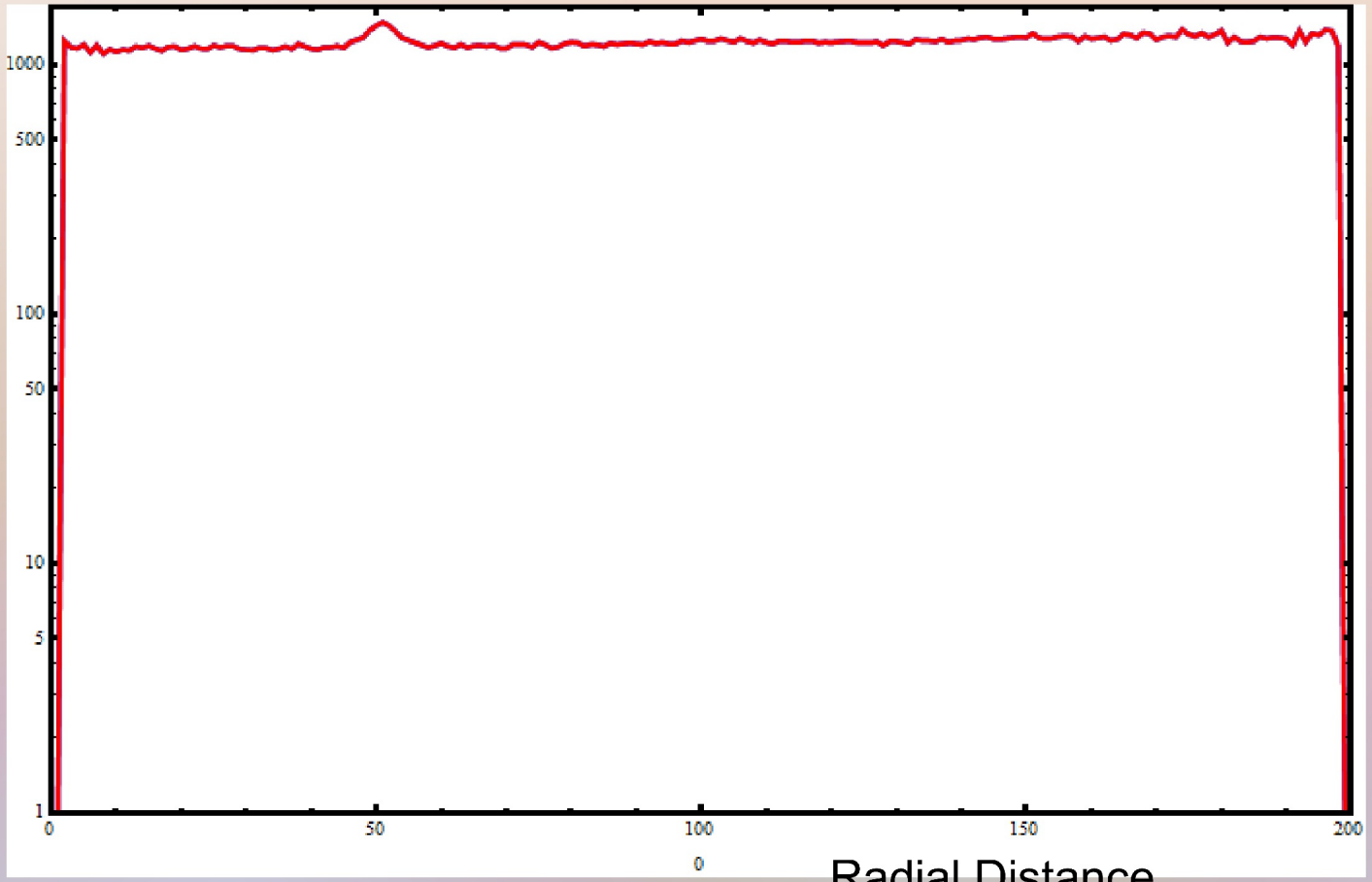
For A = 1/1000, and σ = 1/7 photon, at threshold of 0.44 photons, half the signal if from f_0



Lots of frames

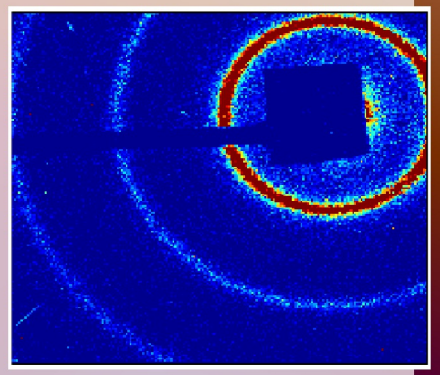
- Integrating detector:
  - few photons per frame
  - using lots of frames → systematics dominate if ignored.
  - thresholding.
    - error in measurement of zero level.
    - photon counting detectors (effectively) do same thing.
  - threshold level, noise, gain determine number of false hits/detection efficiency.
    - **Trade-off**: effective contrast ↔ detection efficiency

Varying Threshold



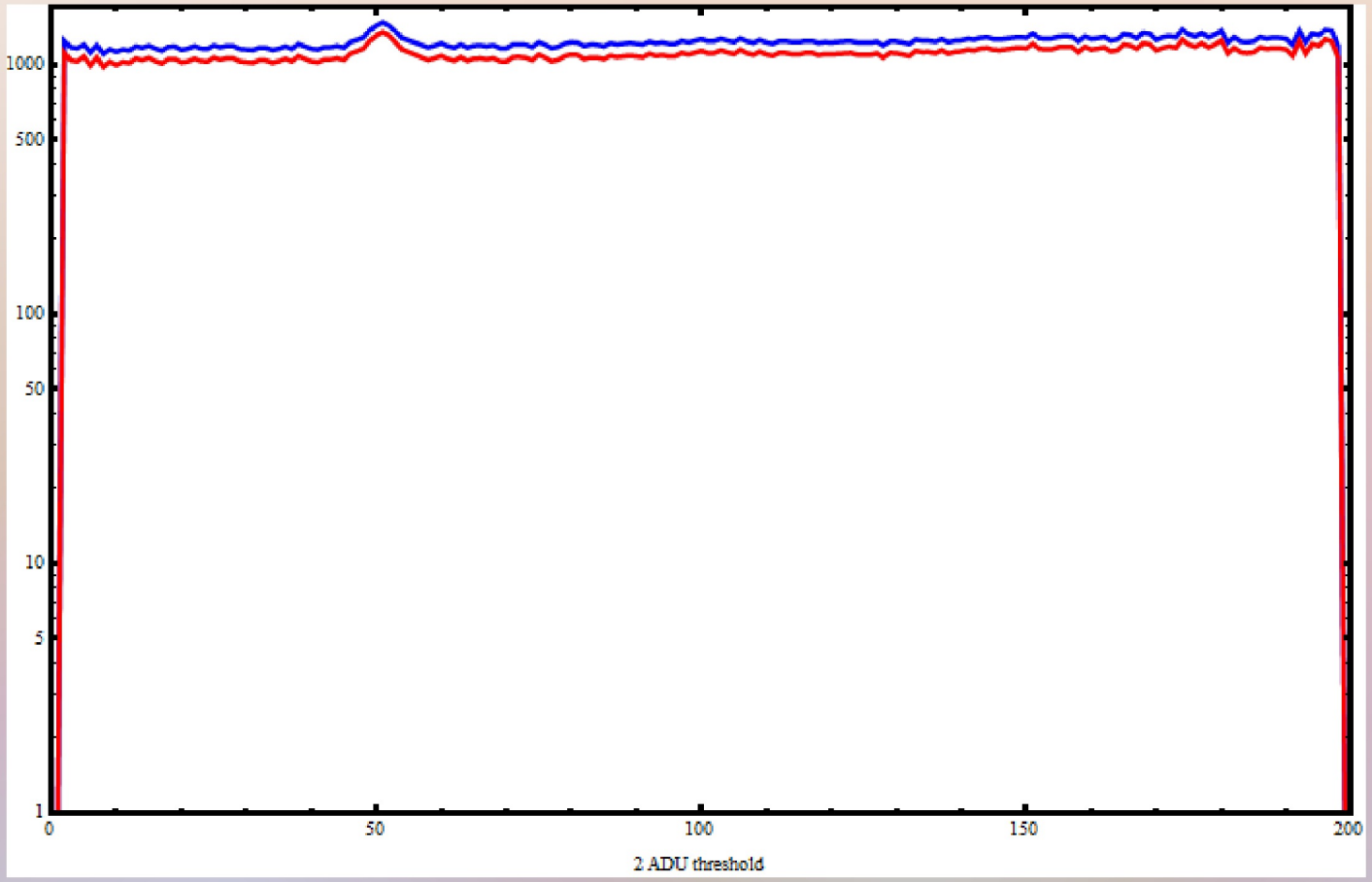
~ 20 ADU/x-ray

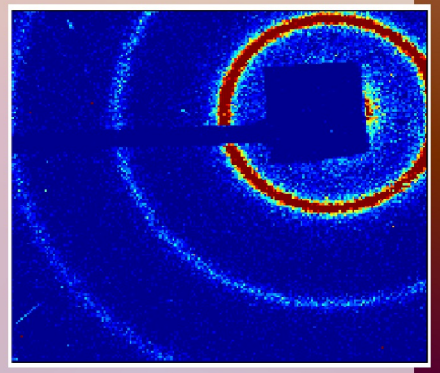
1000 frame sum



(Azimuthal integration around detector)

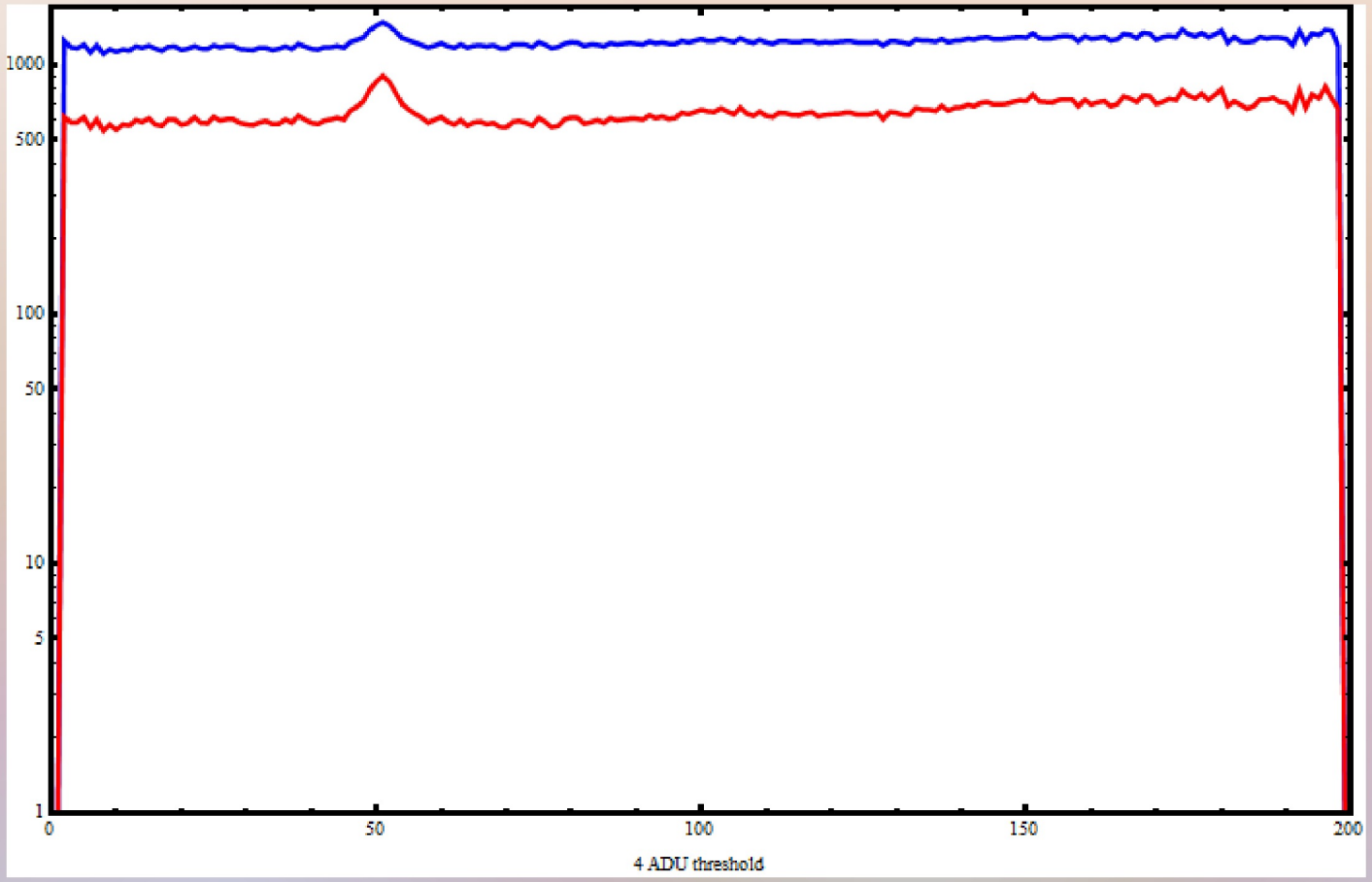
Varying Threshold

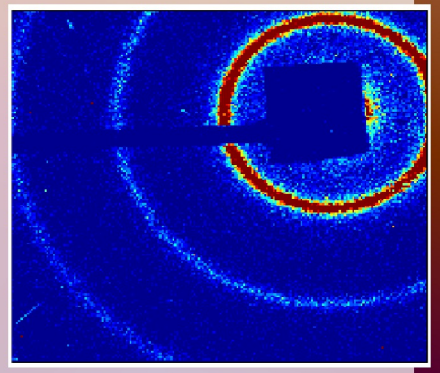




(Azimuthal integration around detector)

Varying Threshold





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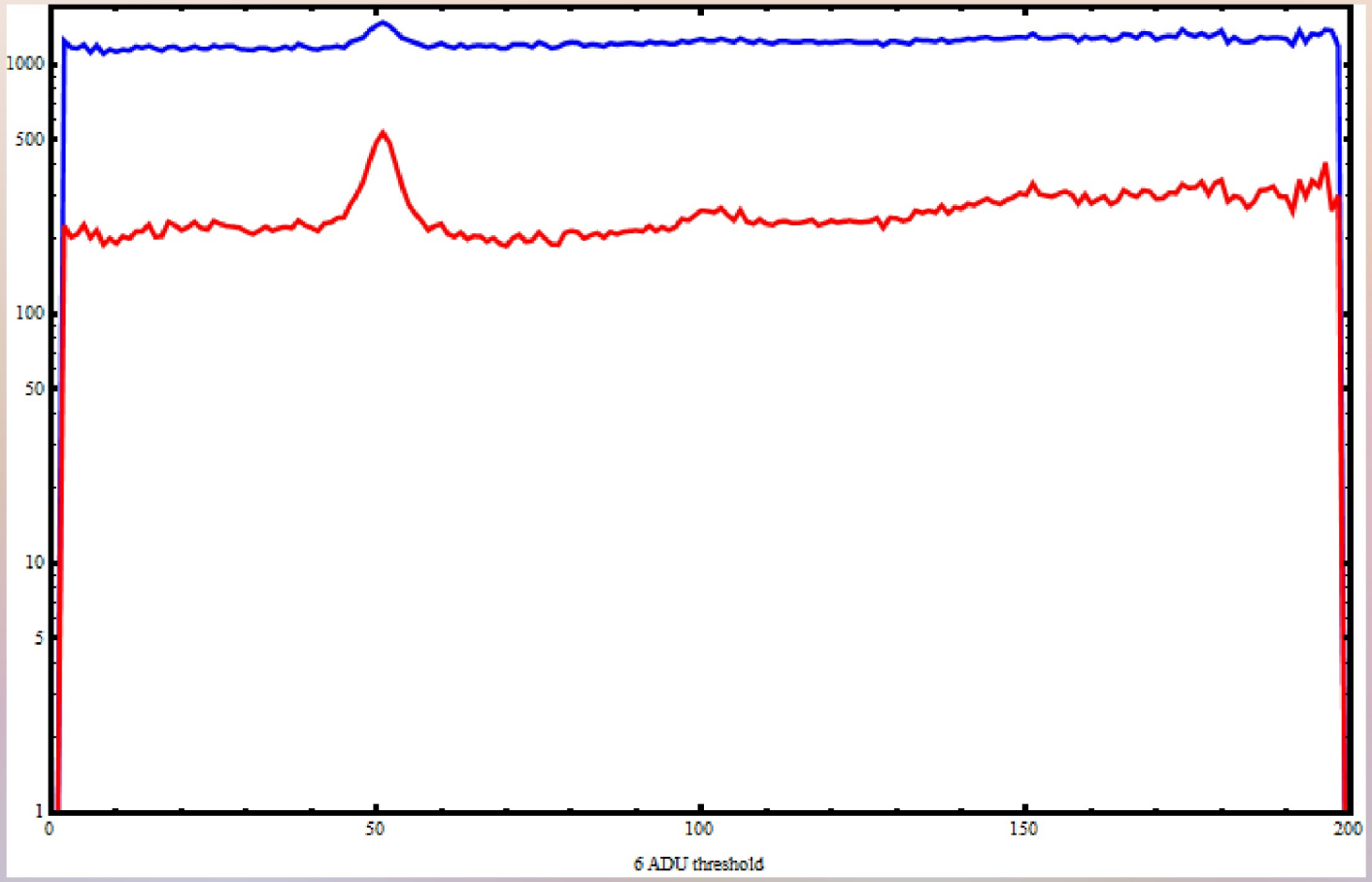
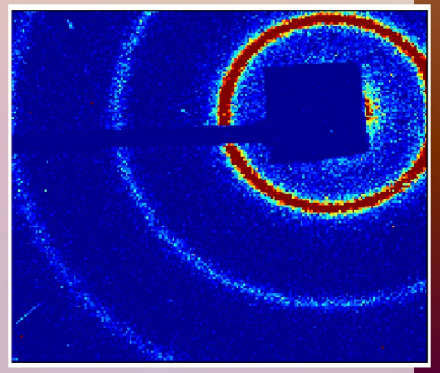
Varying Threshold





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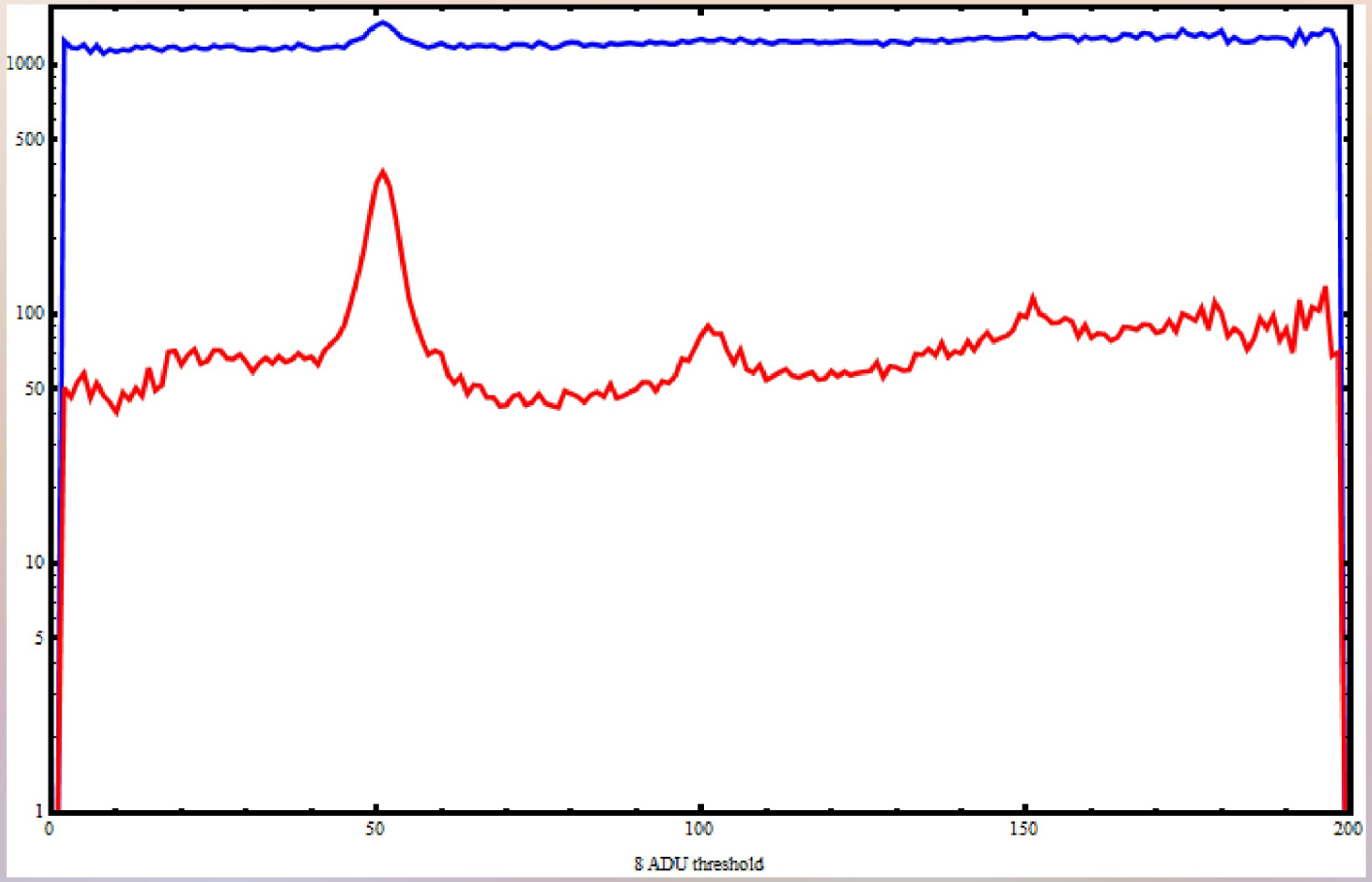
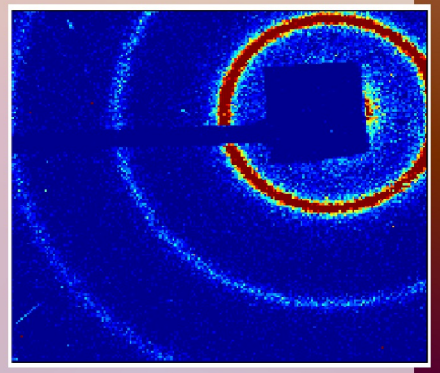
Varying Threshold





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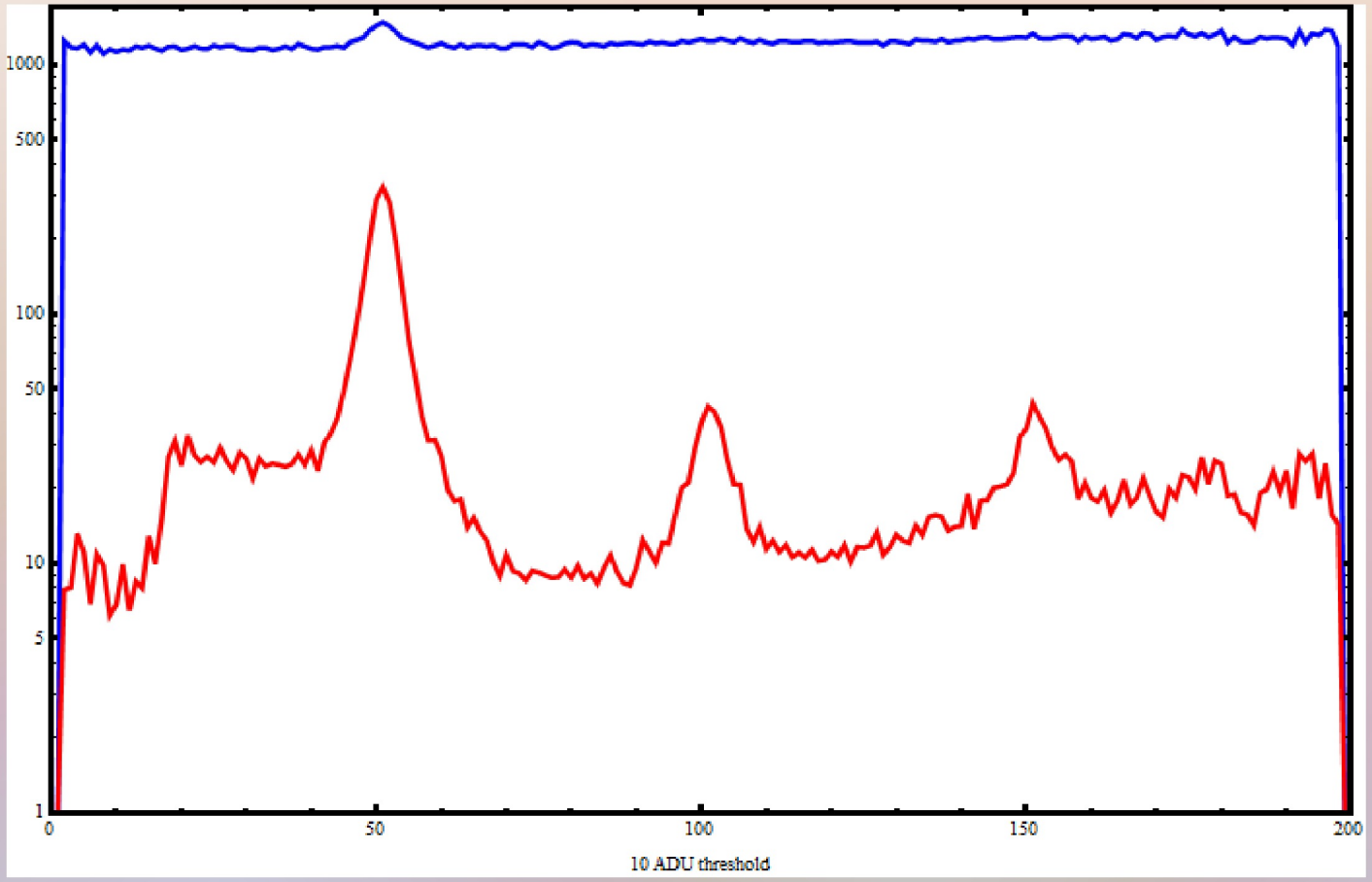
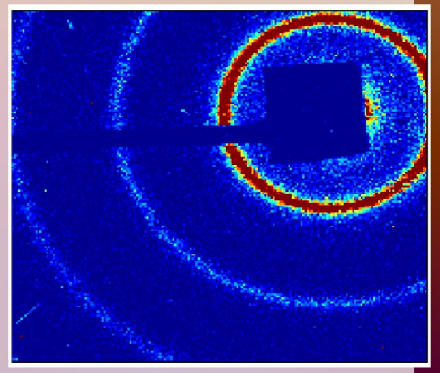
Varying Threshold





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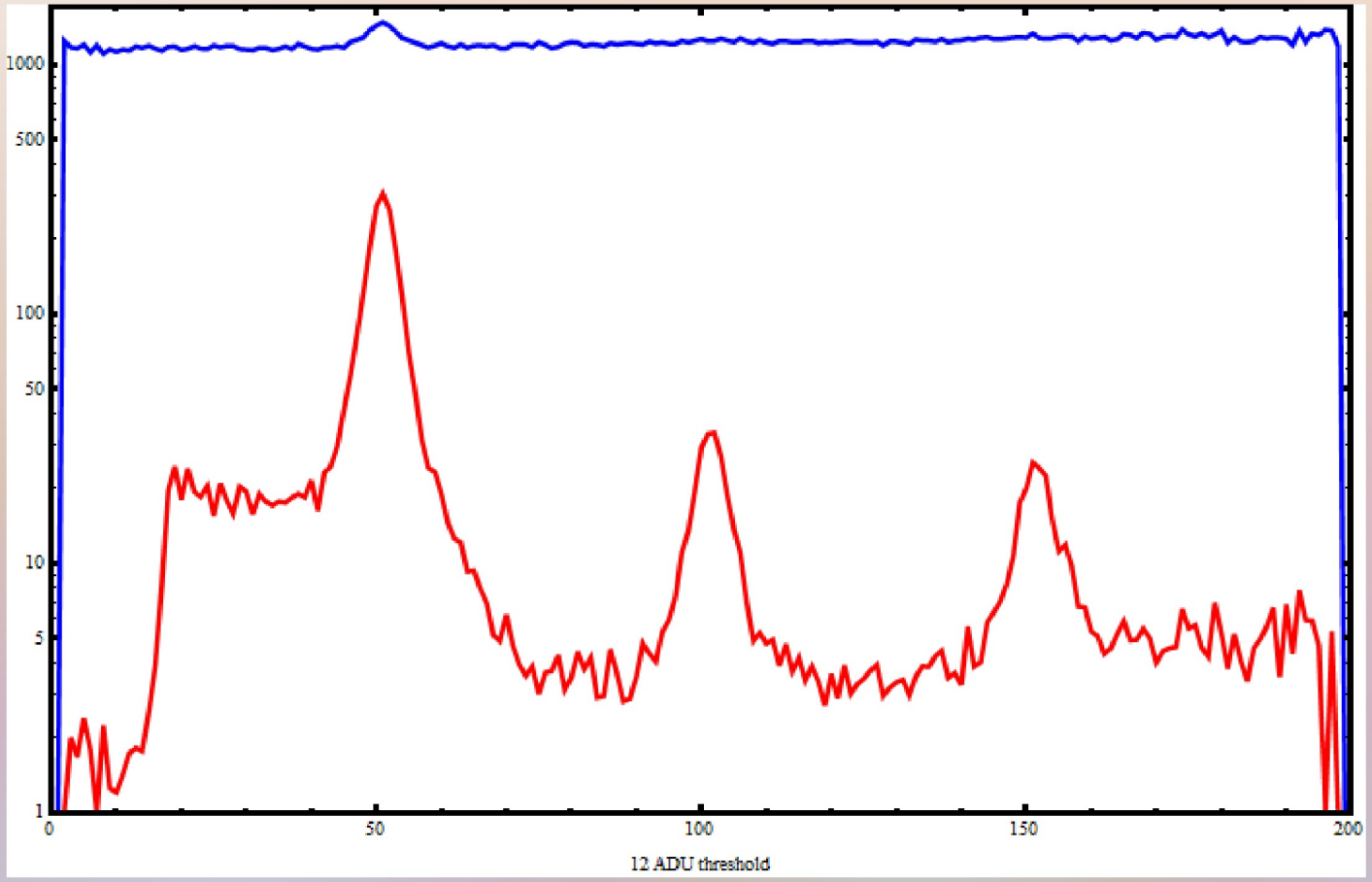

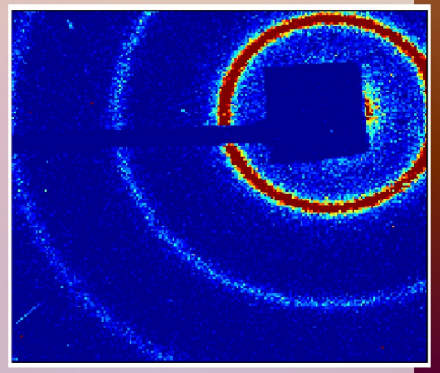

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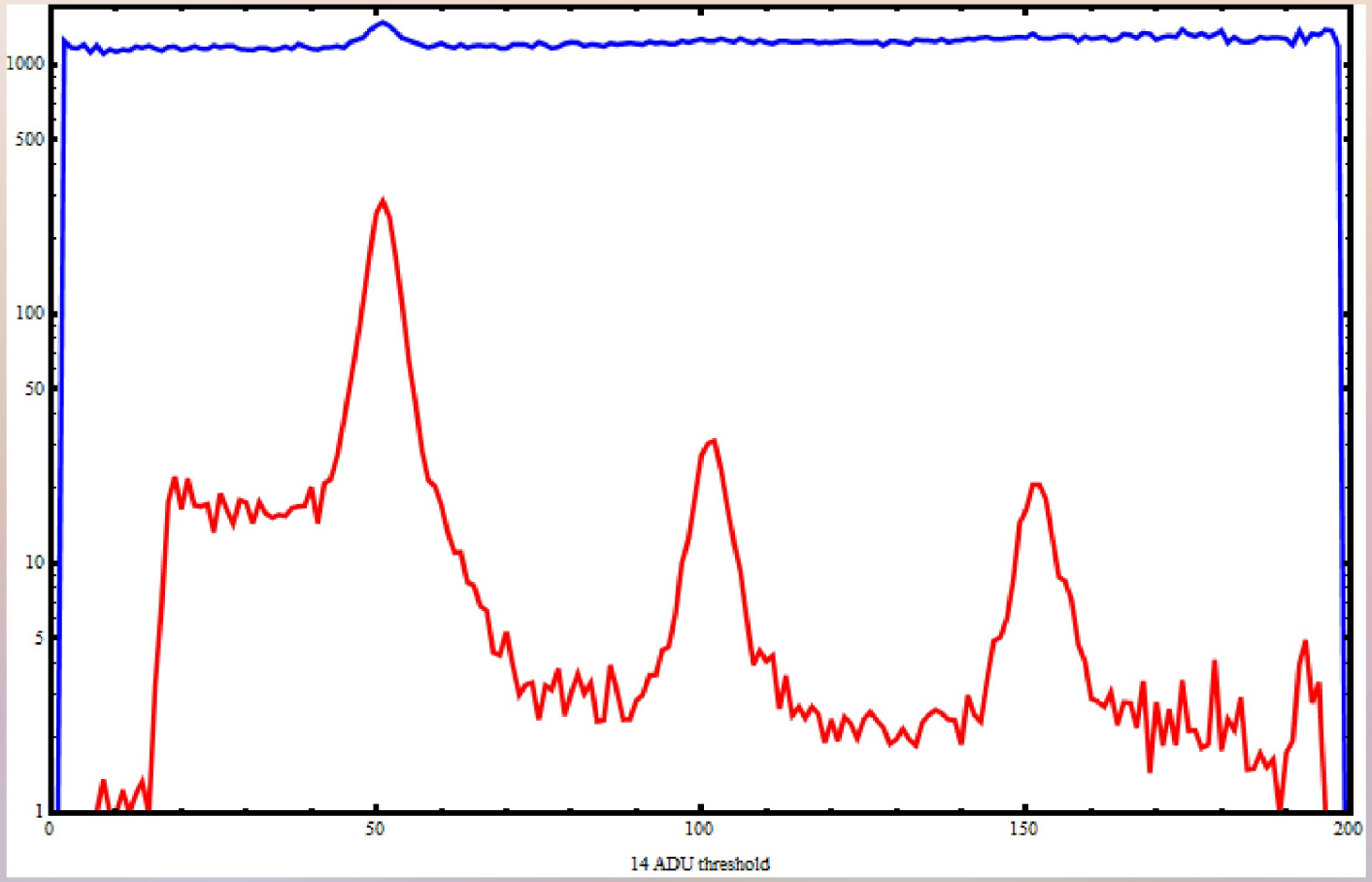
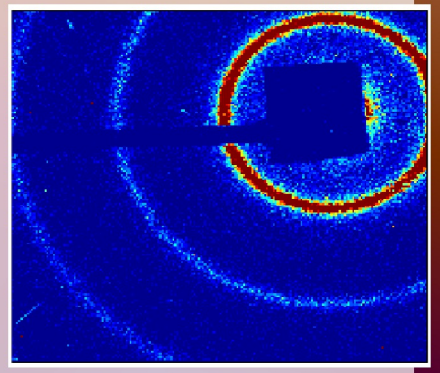
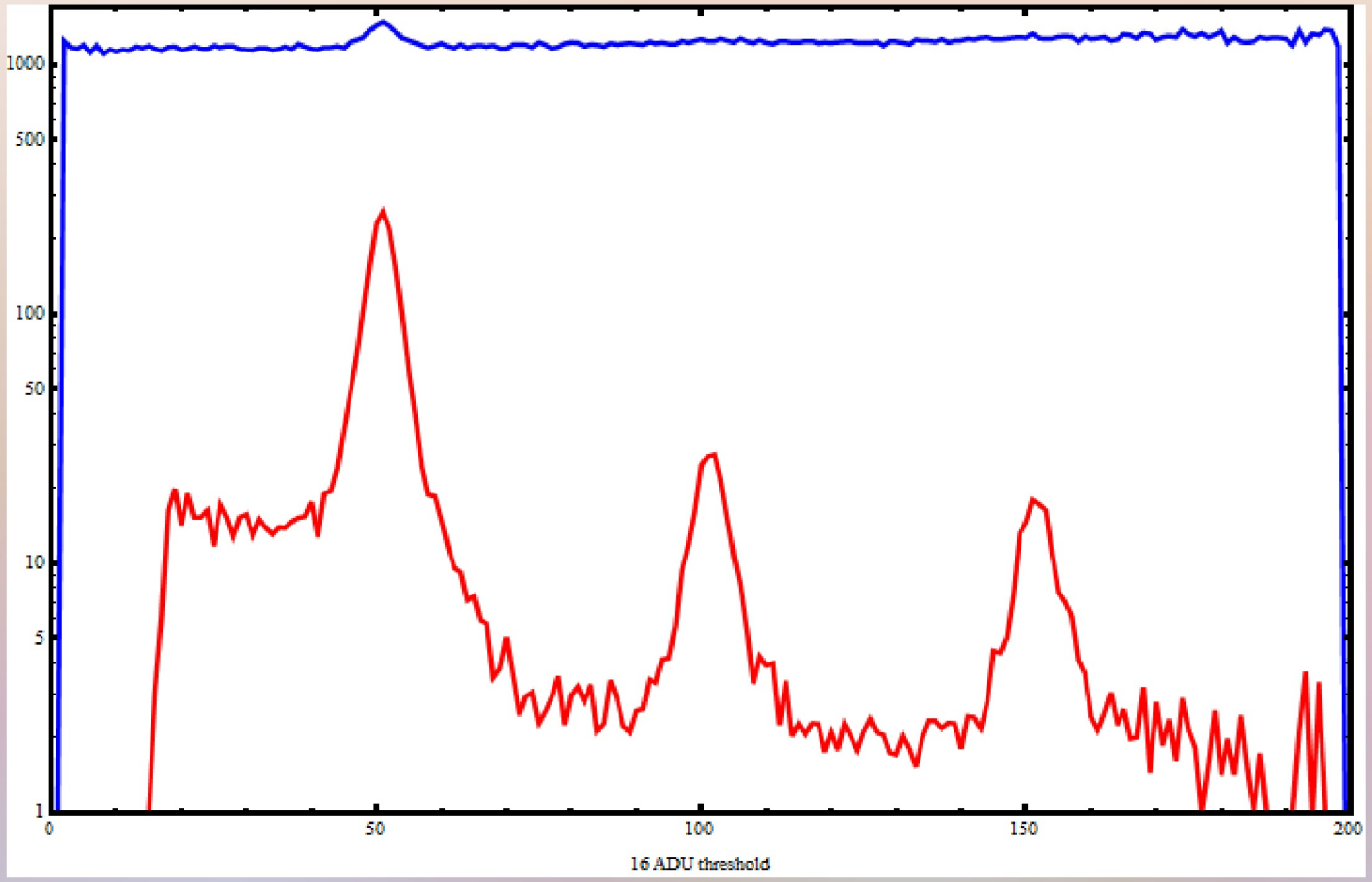
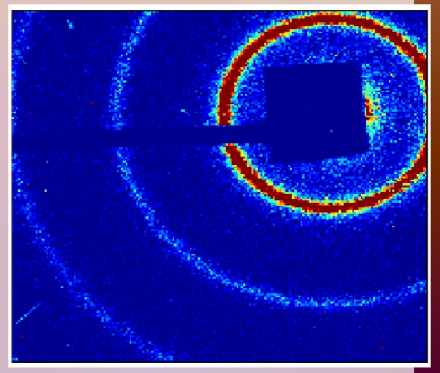




(Azimuthal integration around detector)

Varying Threshold





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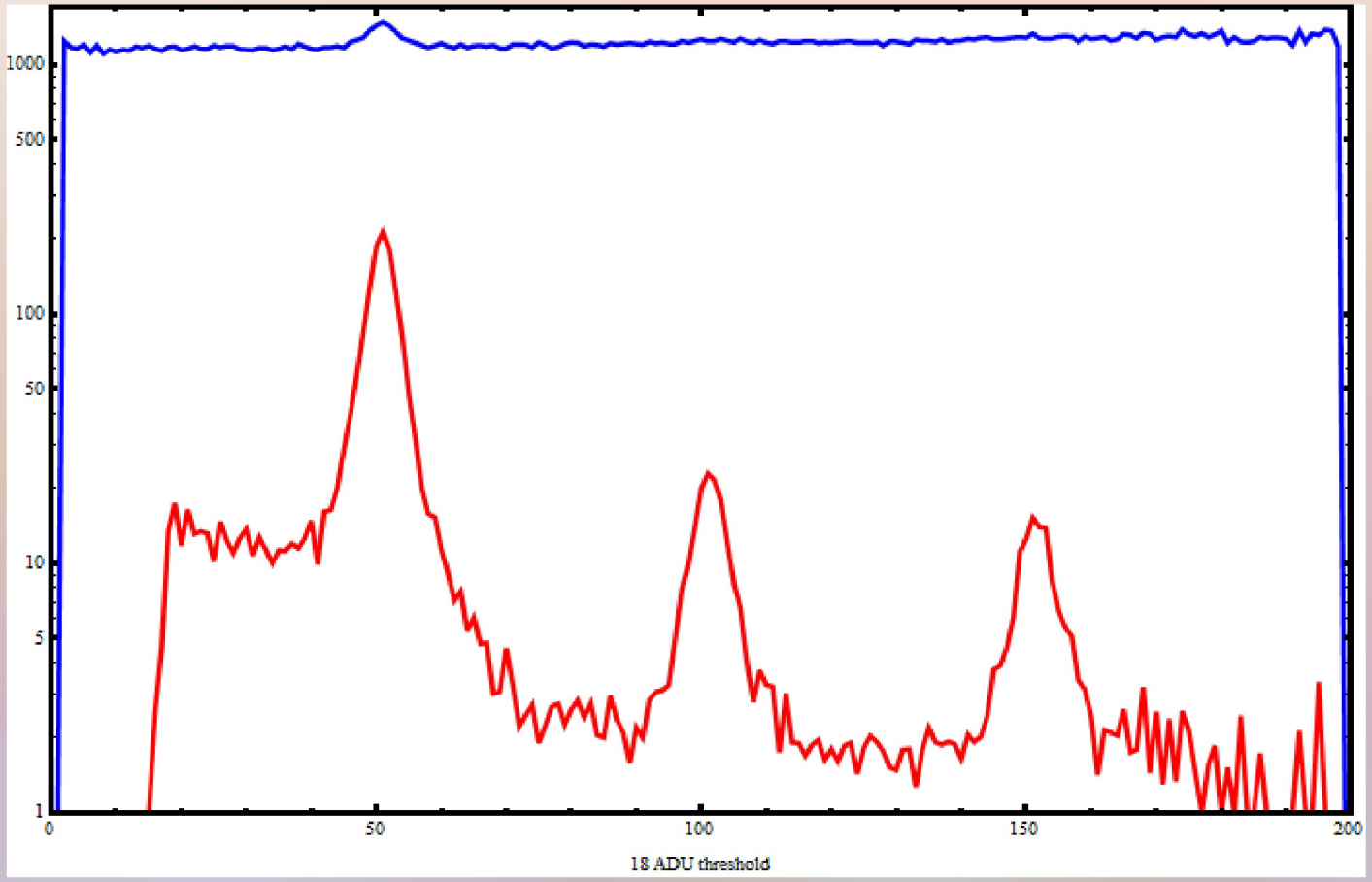
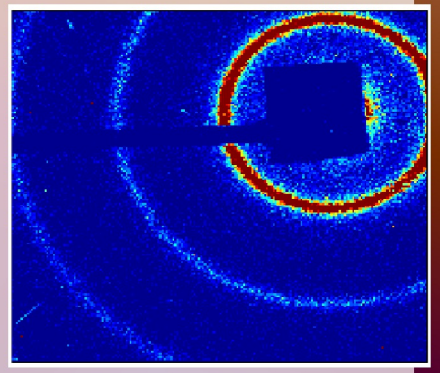
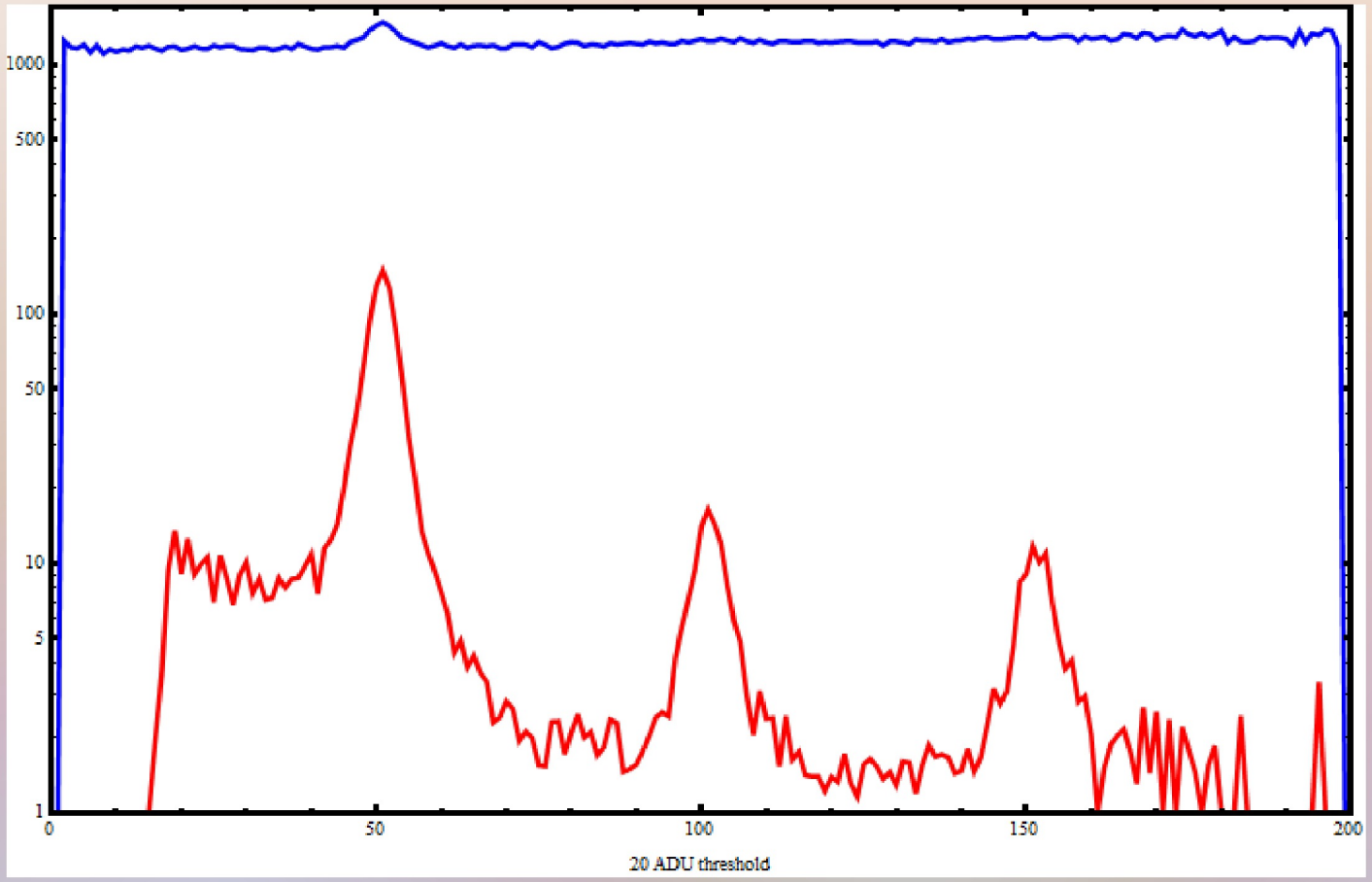
Varying Threshold

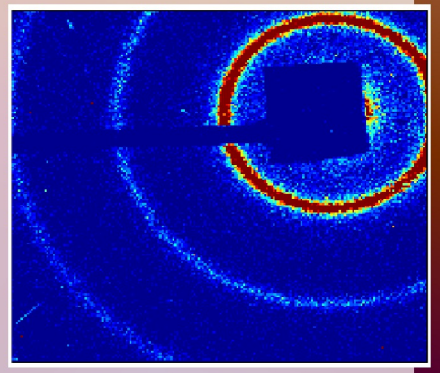




(Azimuthal integration around detector)

Varying Threshold





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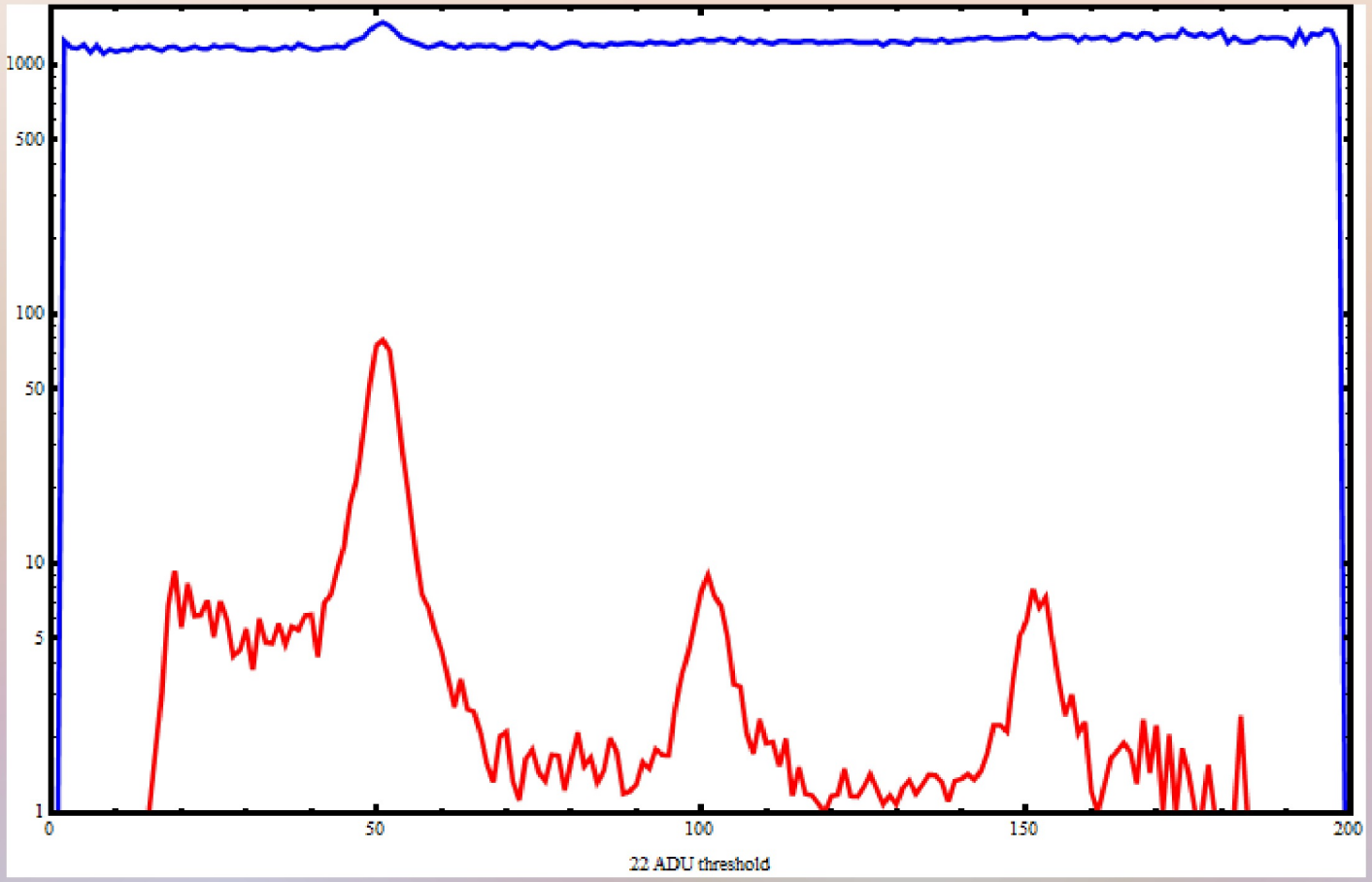
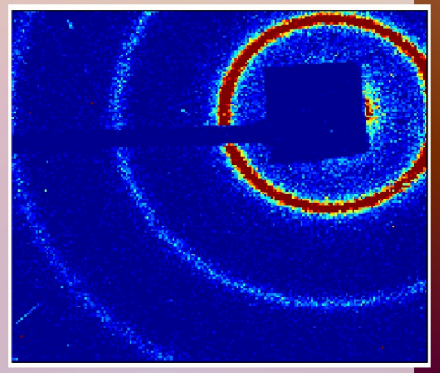
Varying Threshold





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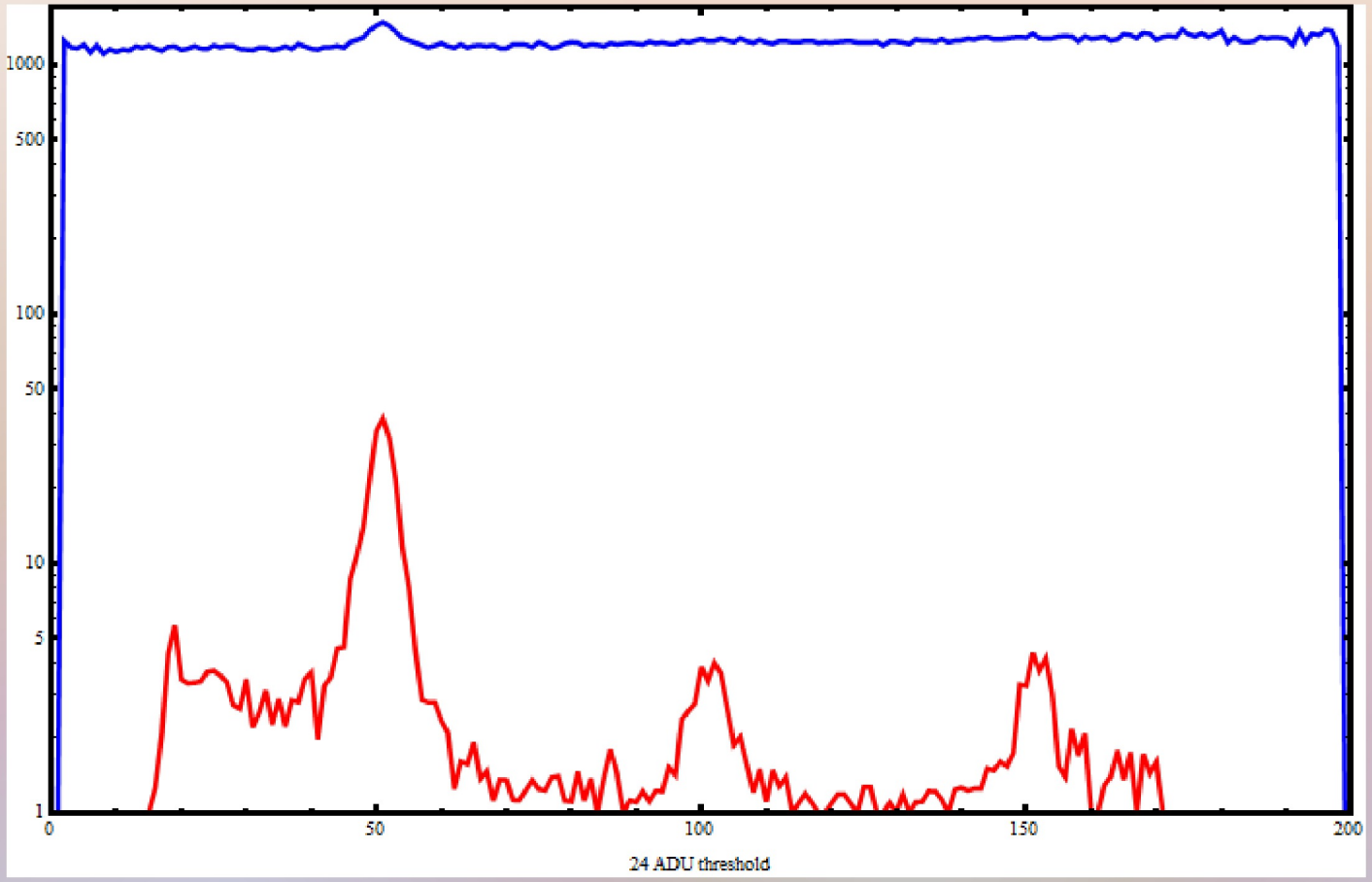
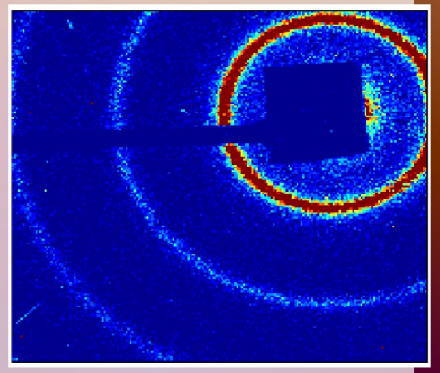
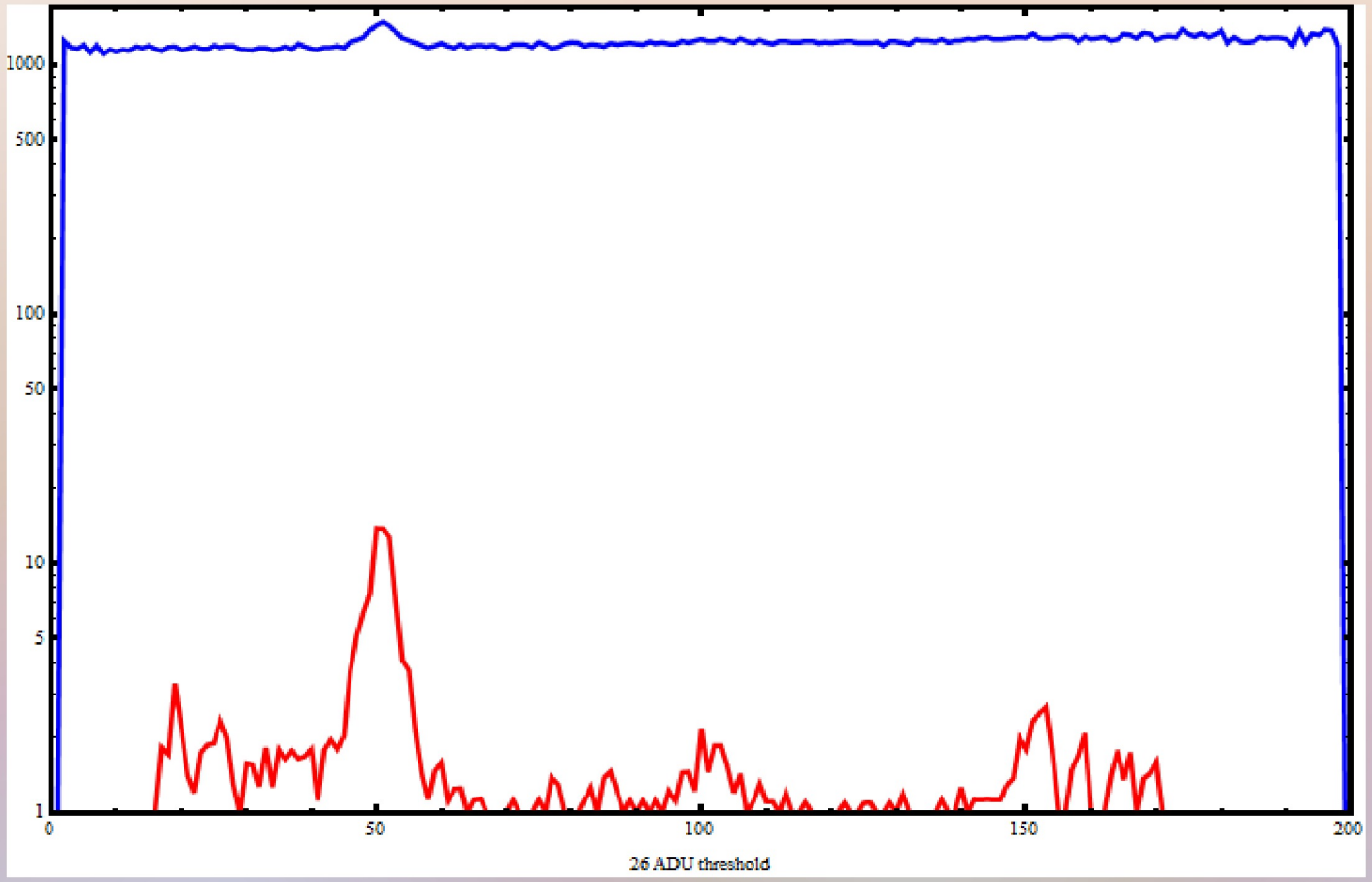
Varying Threshold

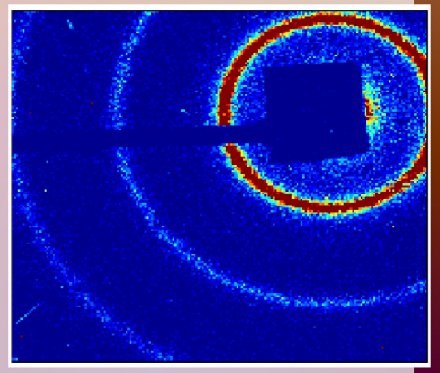




(Azimuthal integration around detector)

Varying Threshold





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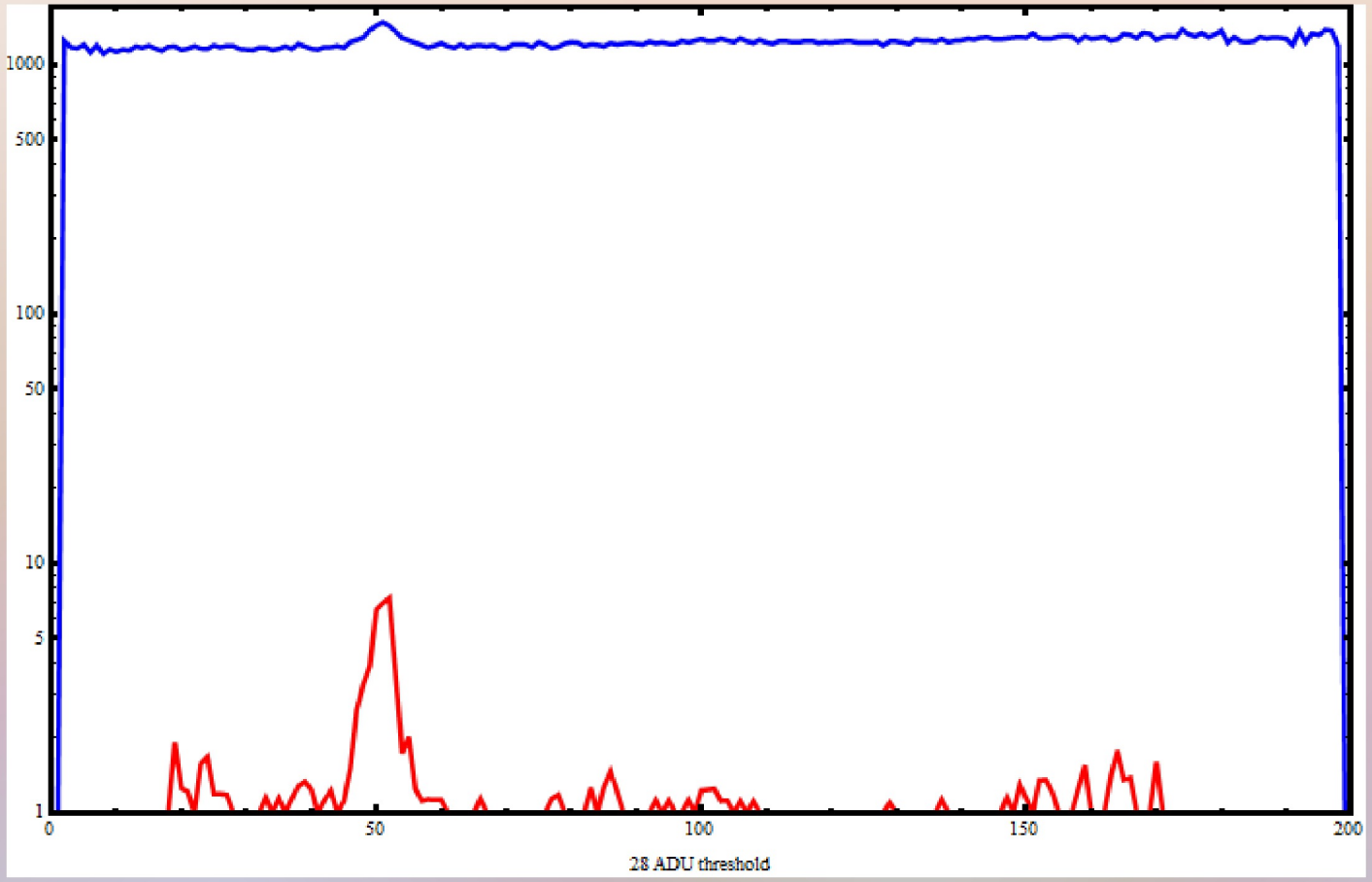
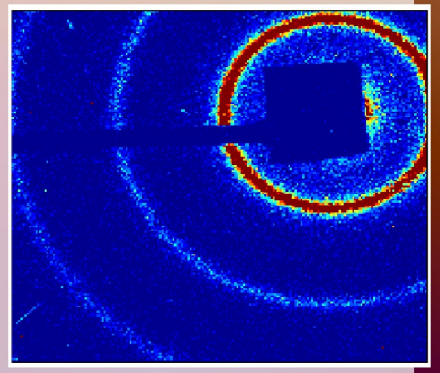
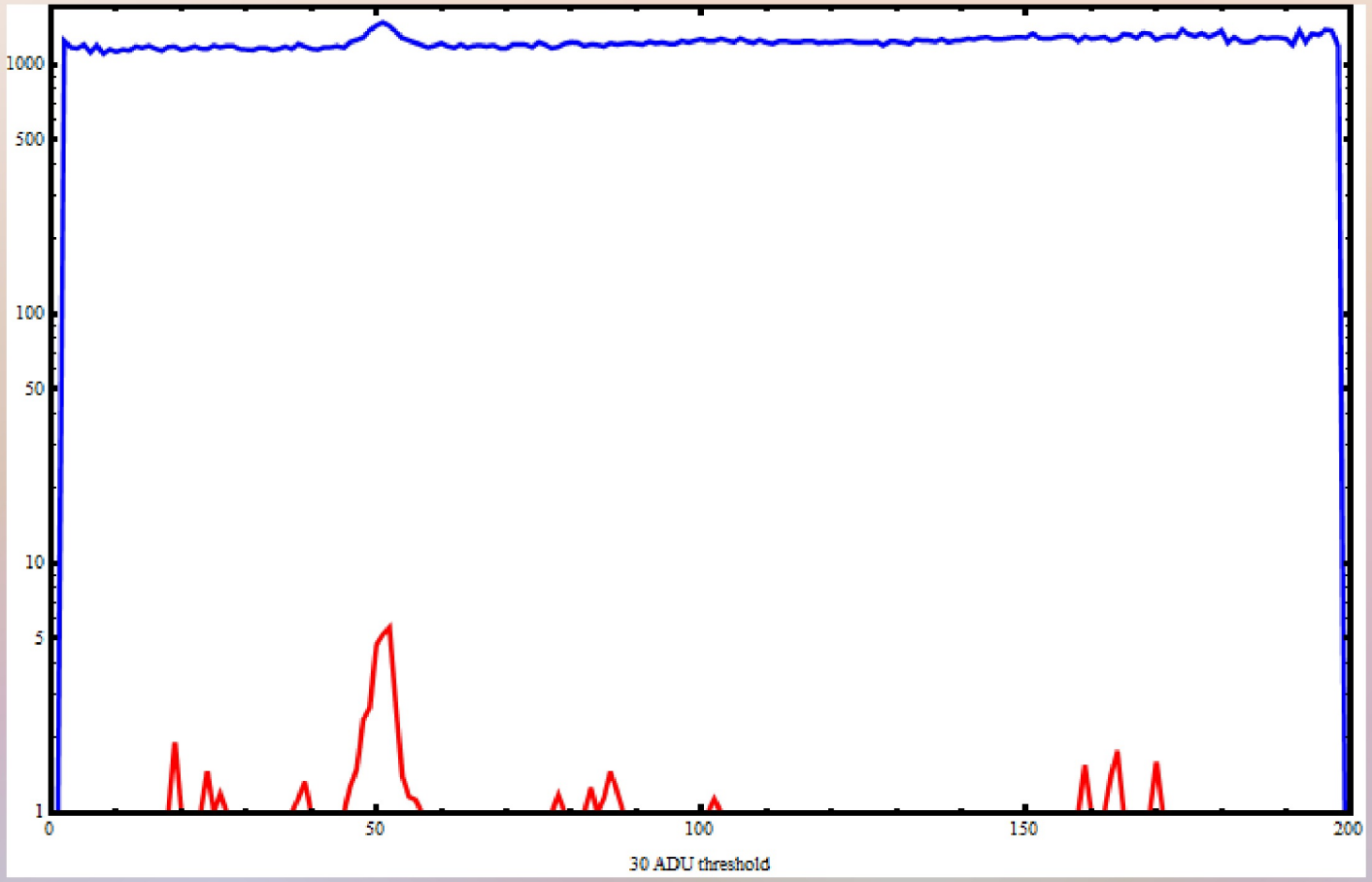
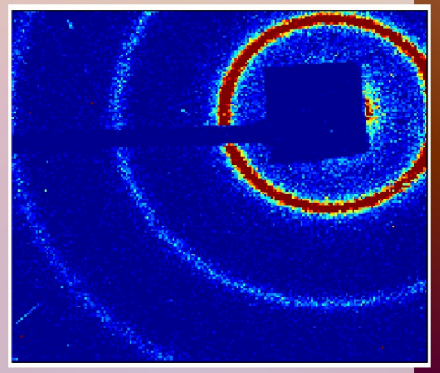




(Azimuthal integration around detector)

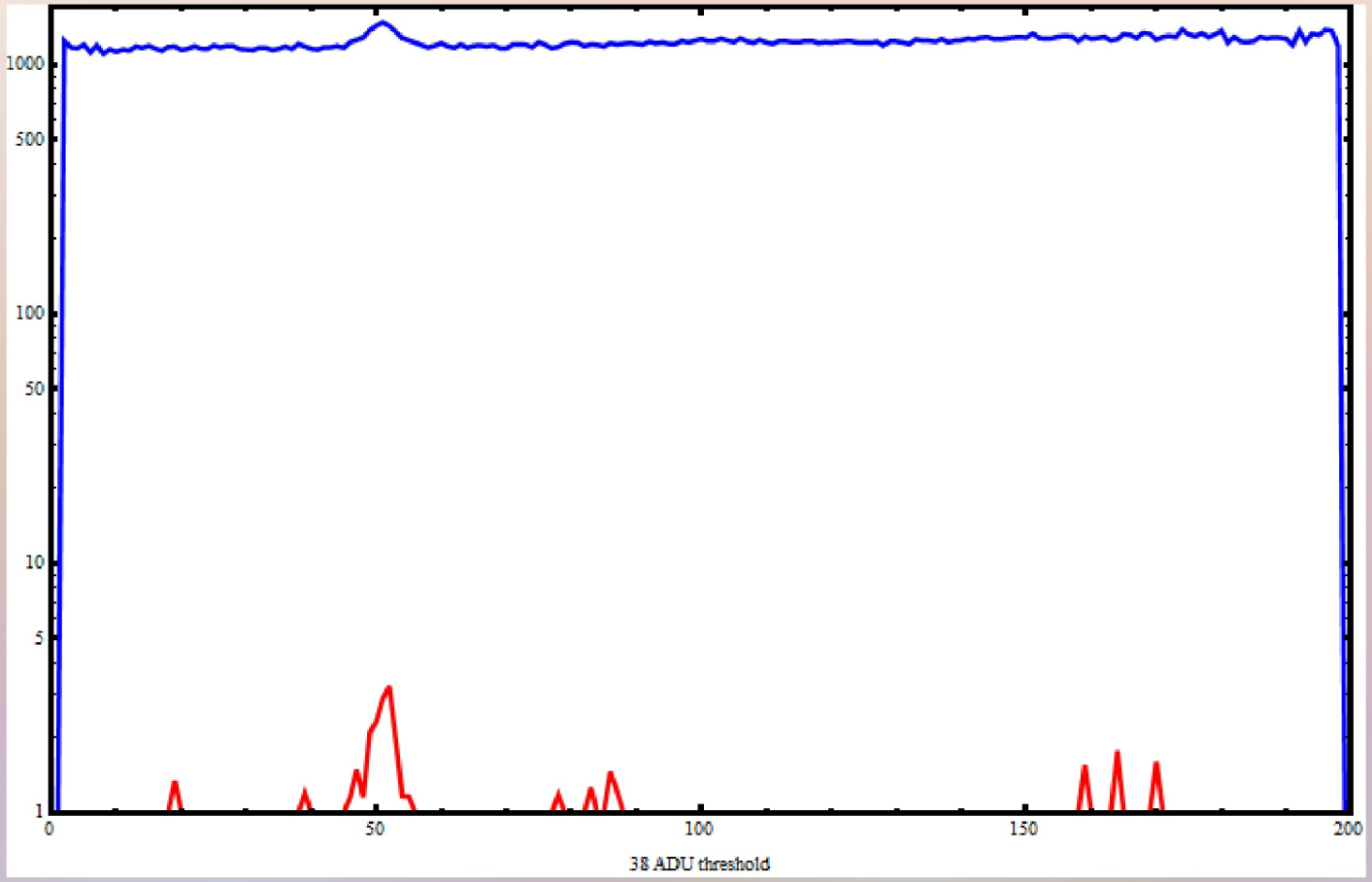
Varying Threshold

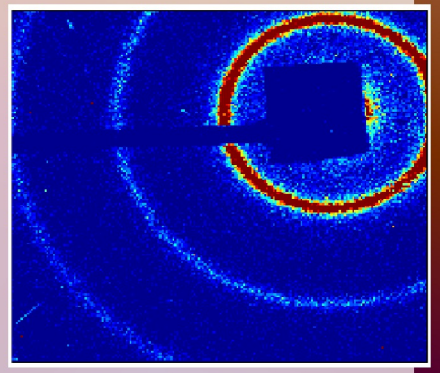




(Azimuthal integration around detector)

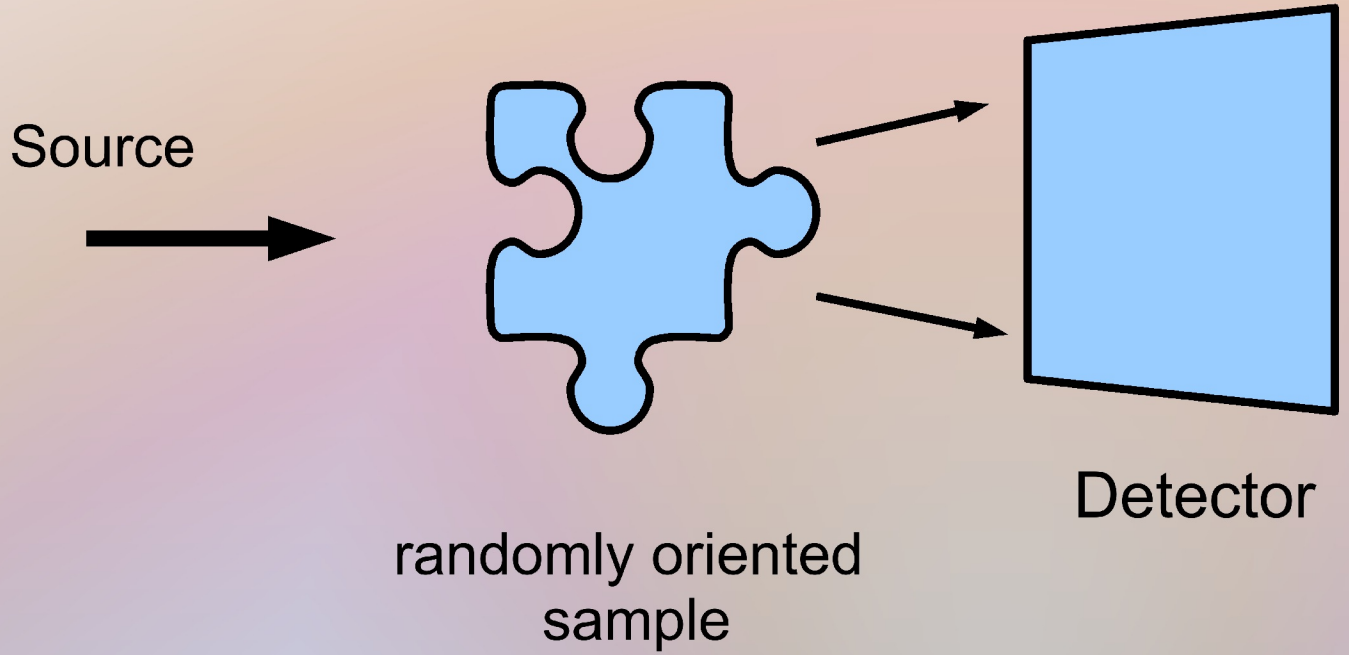
Varying Threshold





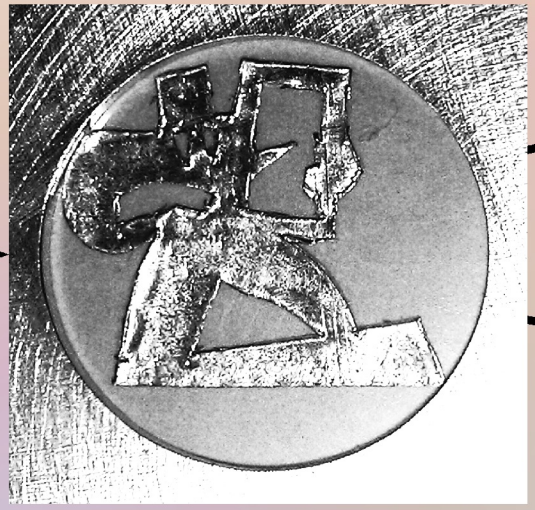
(Azimuthal integration around detector)

Data collection situation

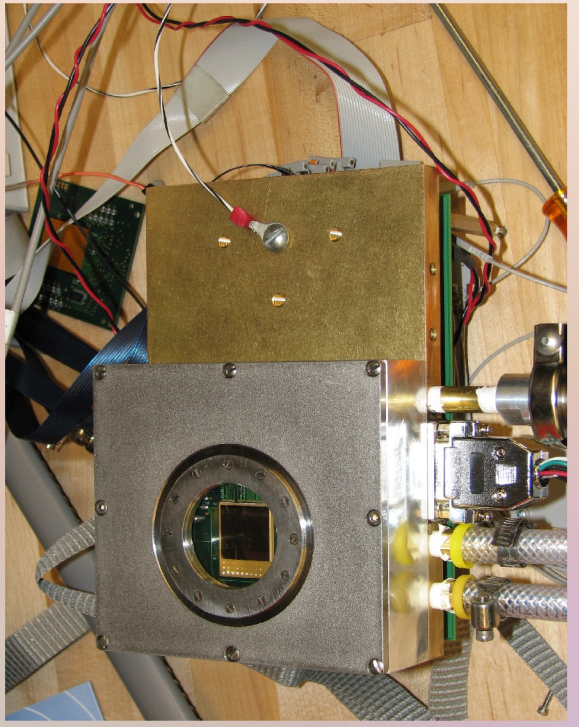


Data collection test

Source



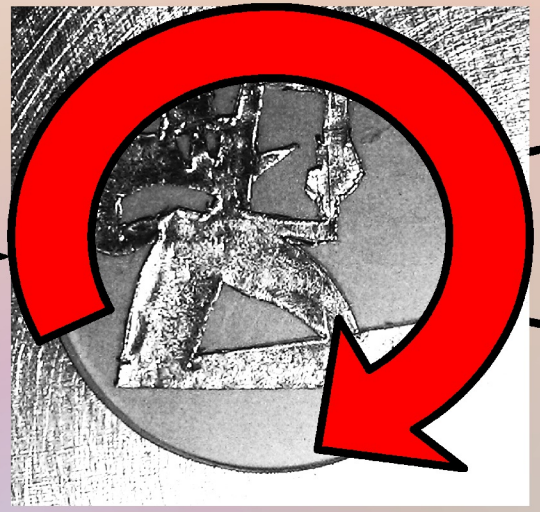
randomly oriented sample



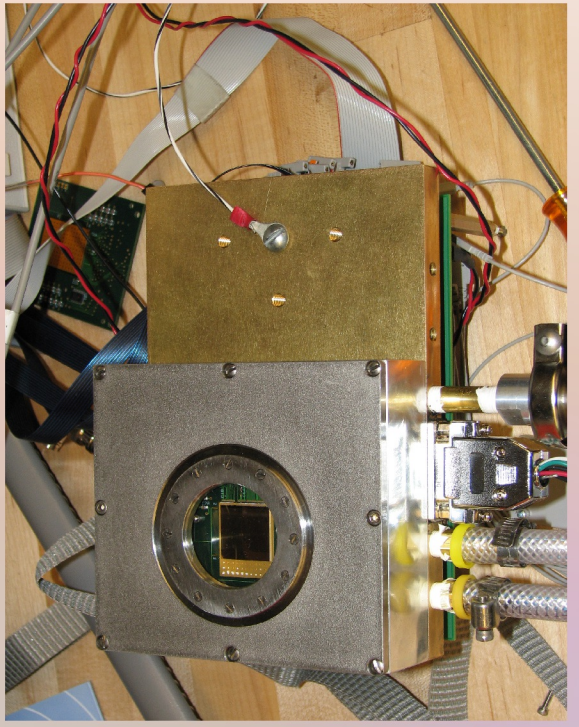
Detector

Data collection test

Source



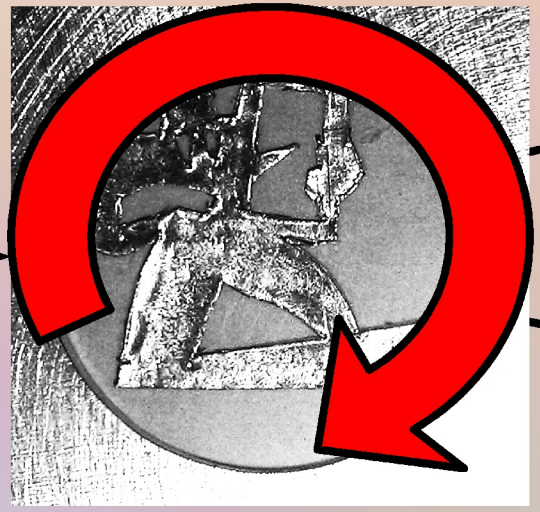
randomly oriented sample



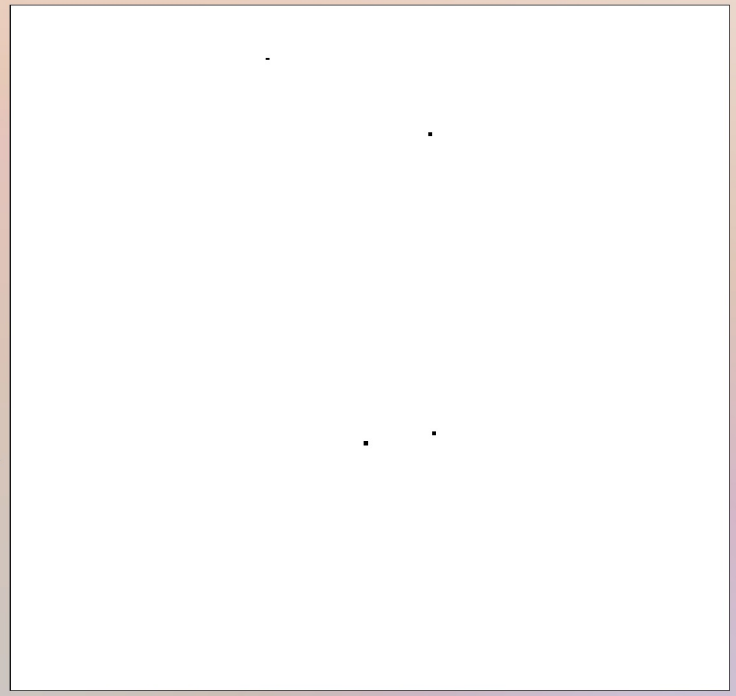
Detector

Data collection test

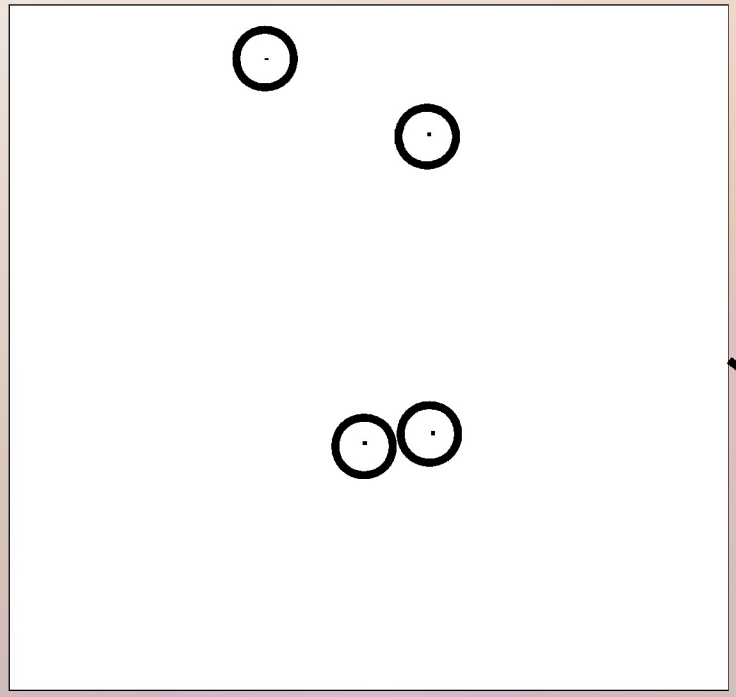
Source



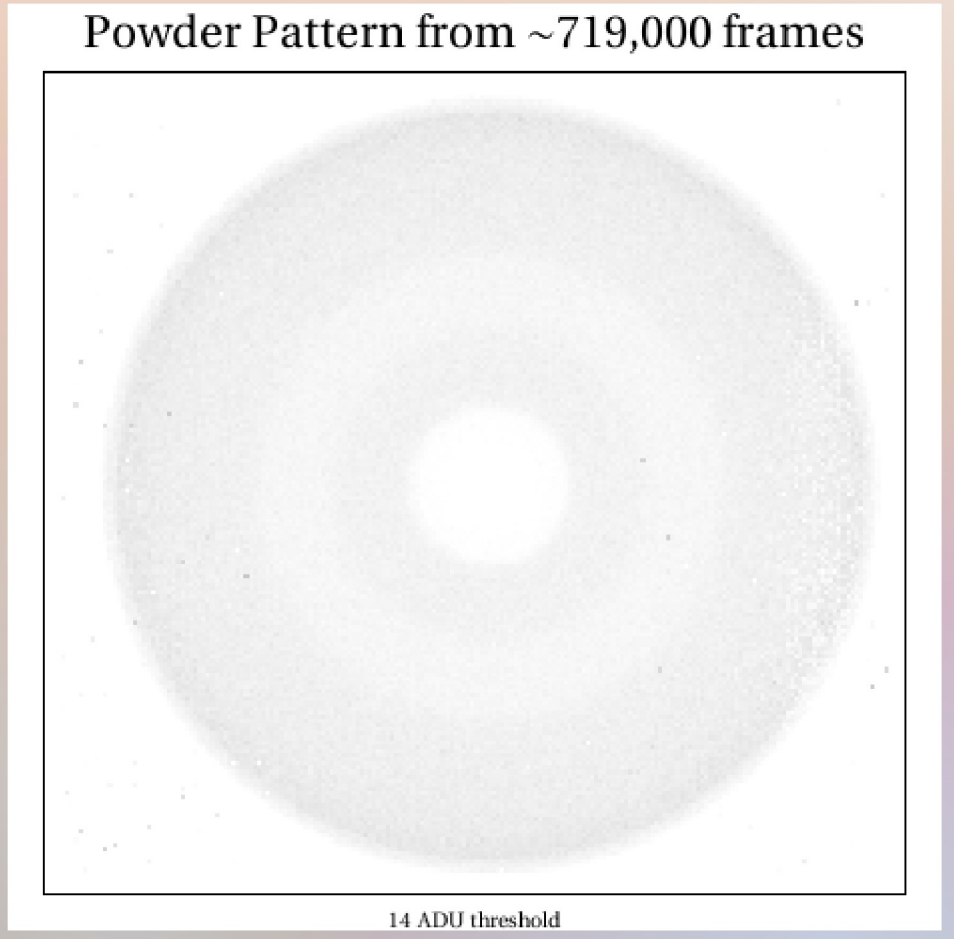
randomly oriented sample



Adding frames



Thresholded Data

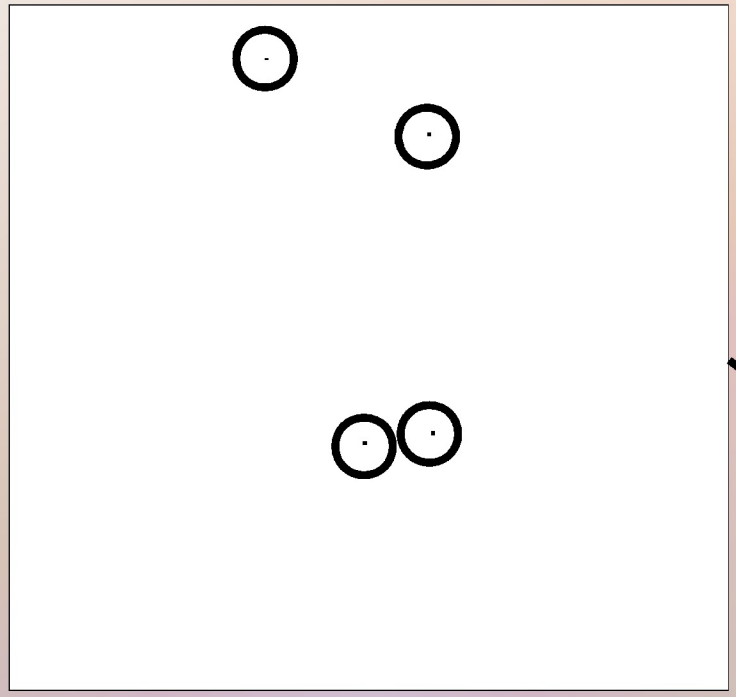


1 8-keV x-ray ~ 20ADU

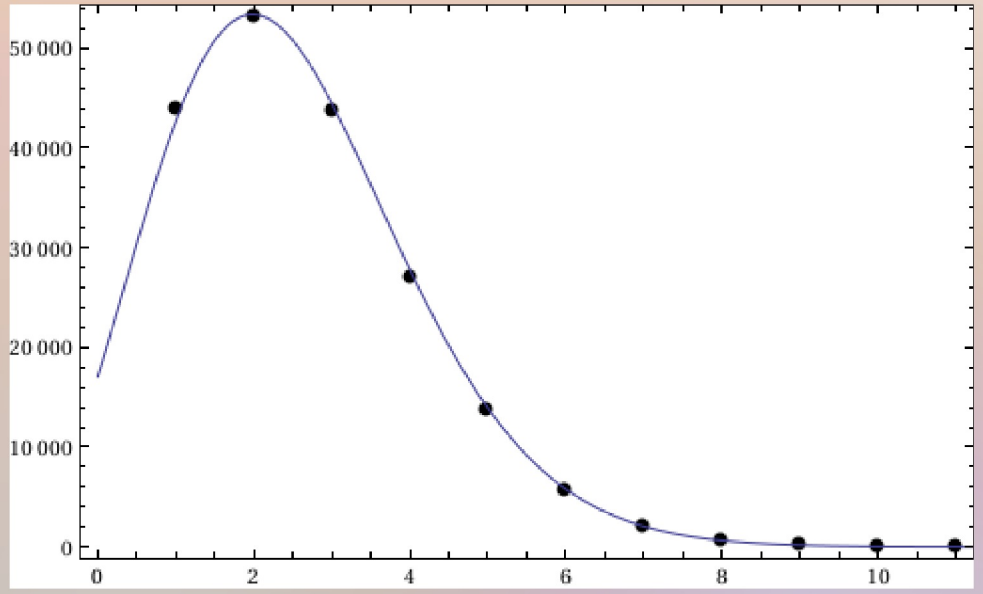
H. T. Philipp, K. Ayyer, M. W. Tate, V. Elser, and S. M. Gruner, "Solving structure with sparse, randomly-oriented x-ray data," Opt. Express 20, 13129-13137 (2012).

Cornell PAD Development

Adding frames

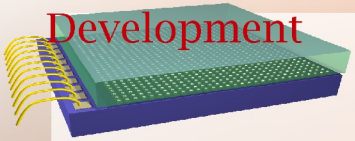


Thresholded Data

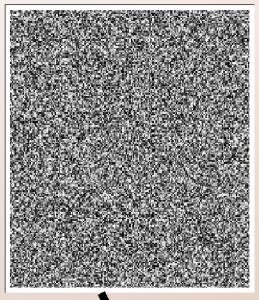


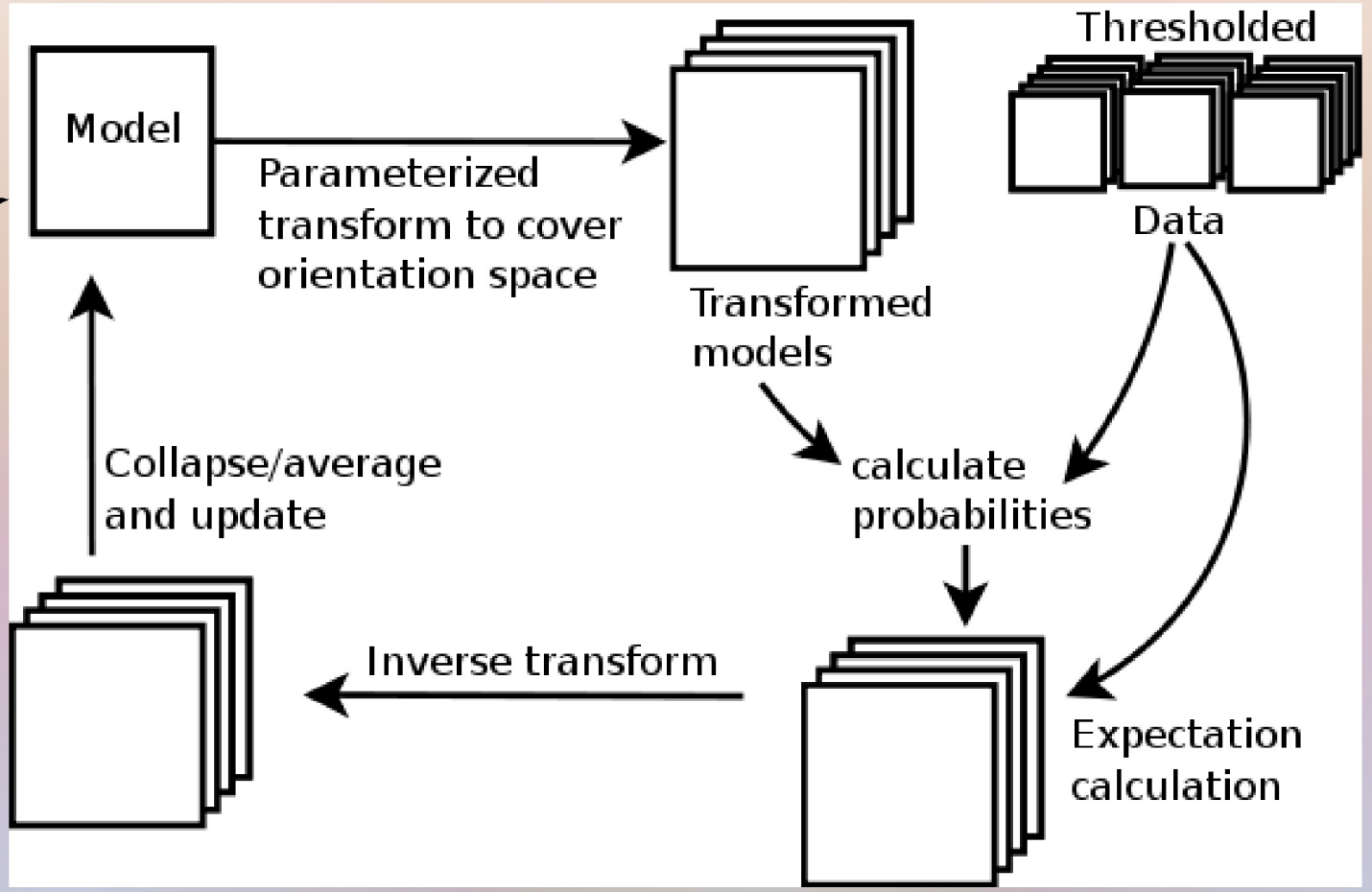
Histogram of x-rays per frame

H. T. Philipp, K. Ayyer, M. W. Tate, V. Elser, and S. M. Gruner, "Solving structure with sparse, randomly-oriented x-ray data," Opt. Express 20, 13129-13137 (2012).

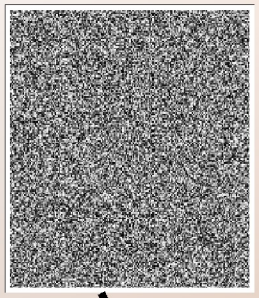


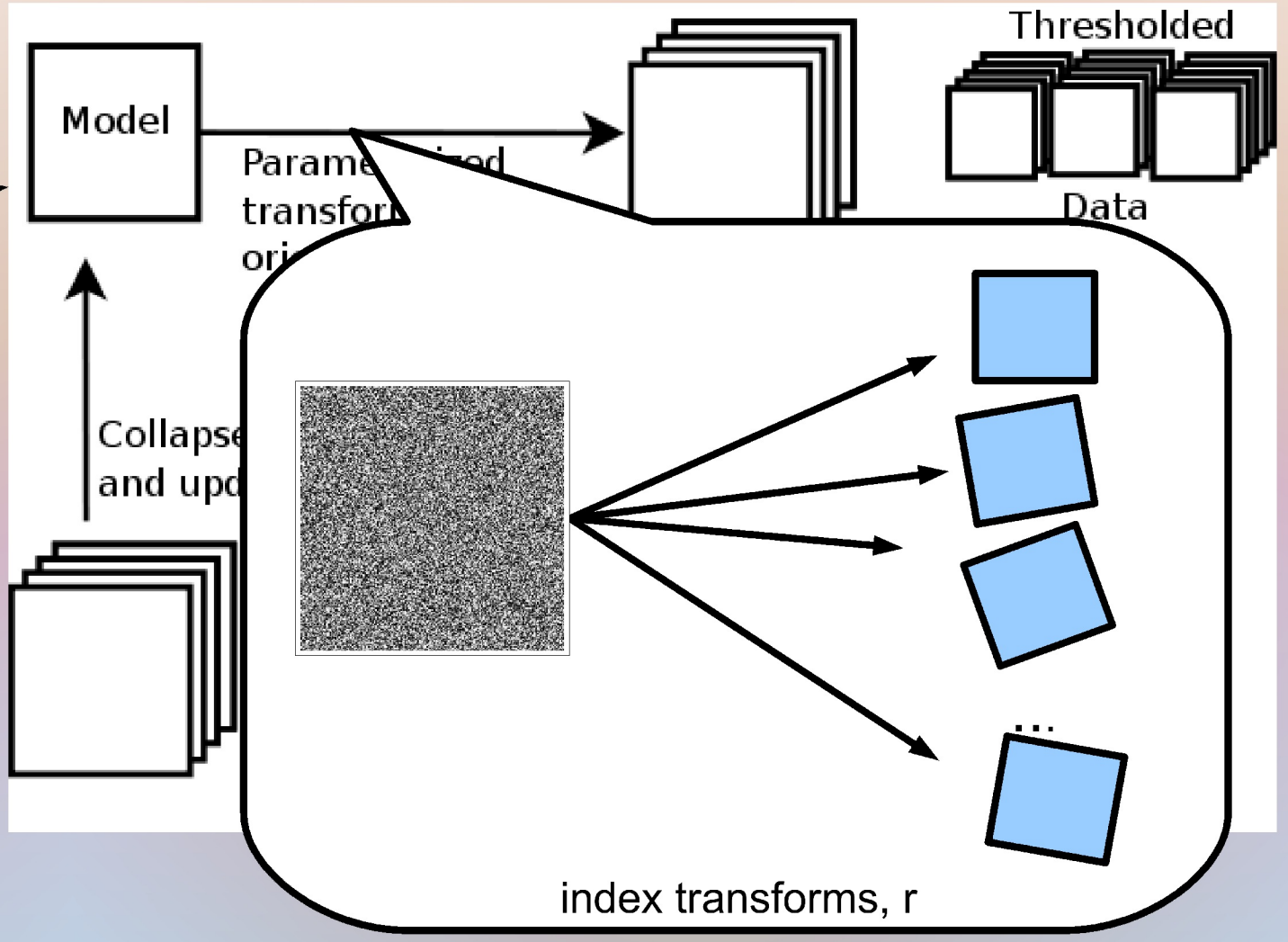
Expectation maximization

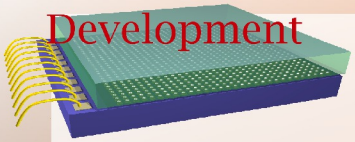


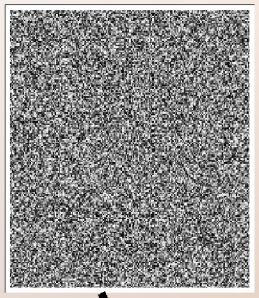


Expectation maximization

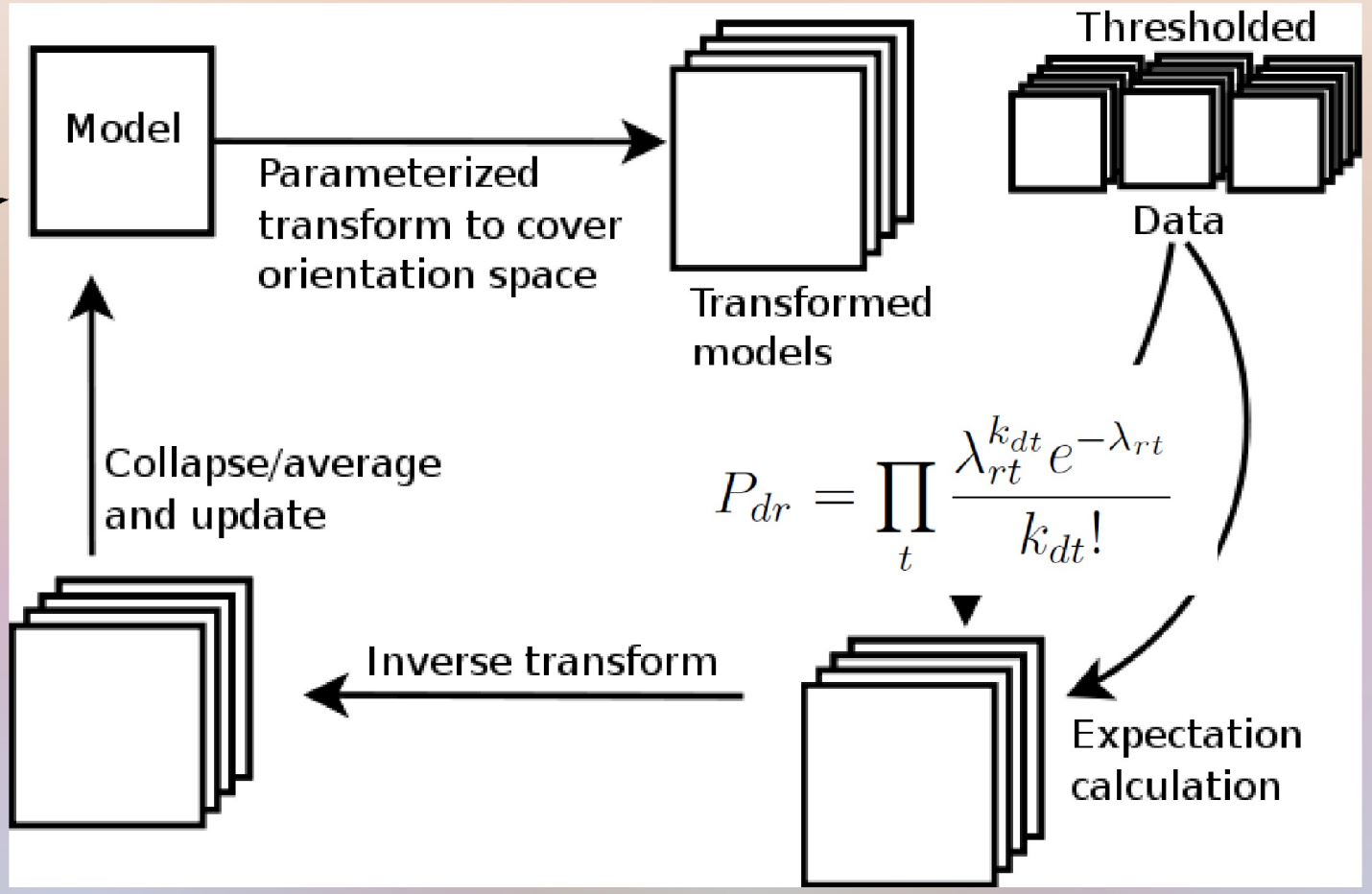






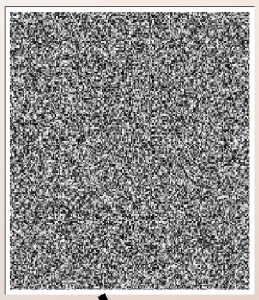


Expectation maximization

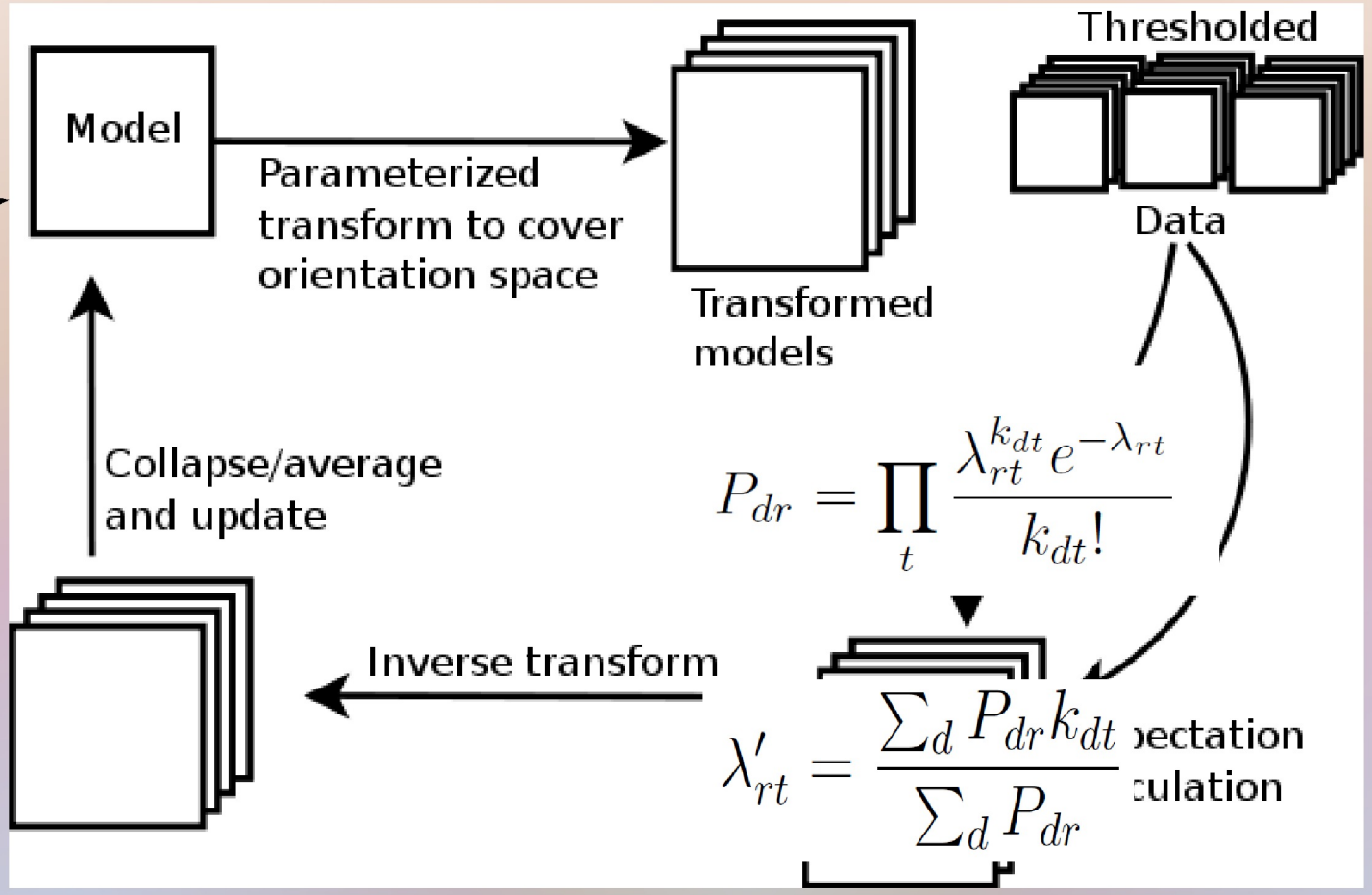


t = pixel index, d = data frame, k = pixel value for data frame, λ = model value

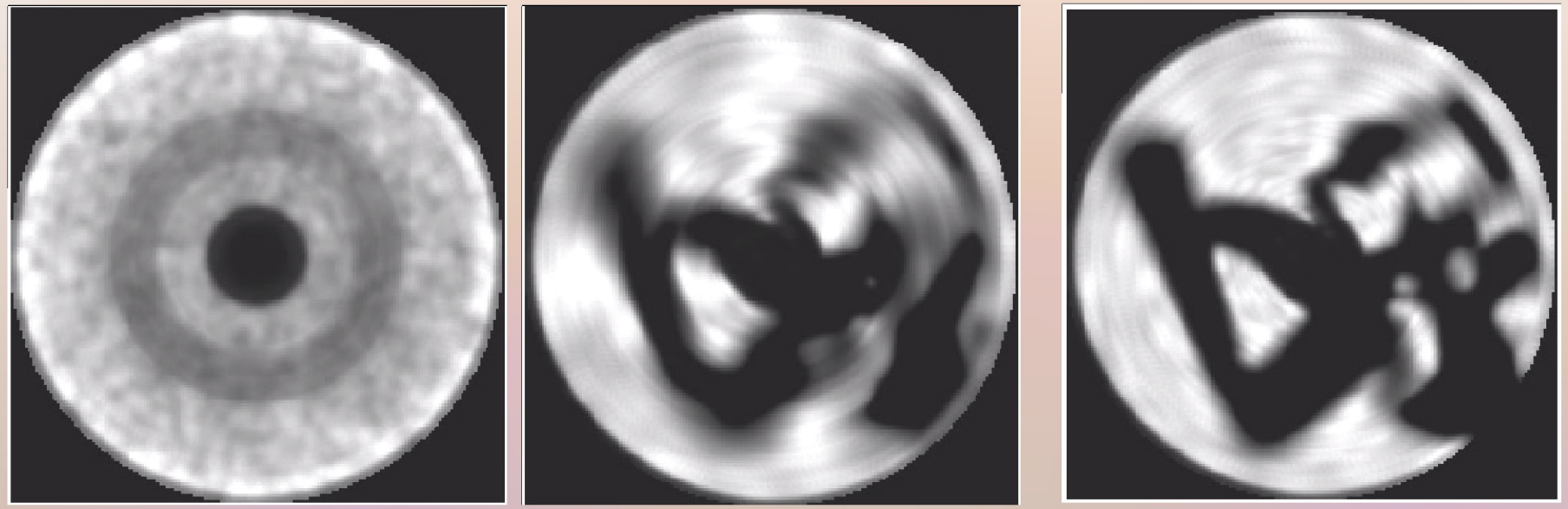
Cornell PAD Development



Expectation maximization



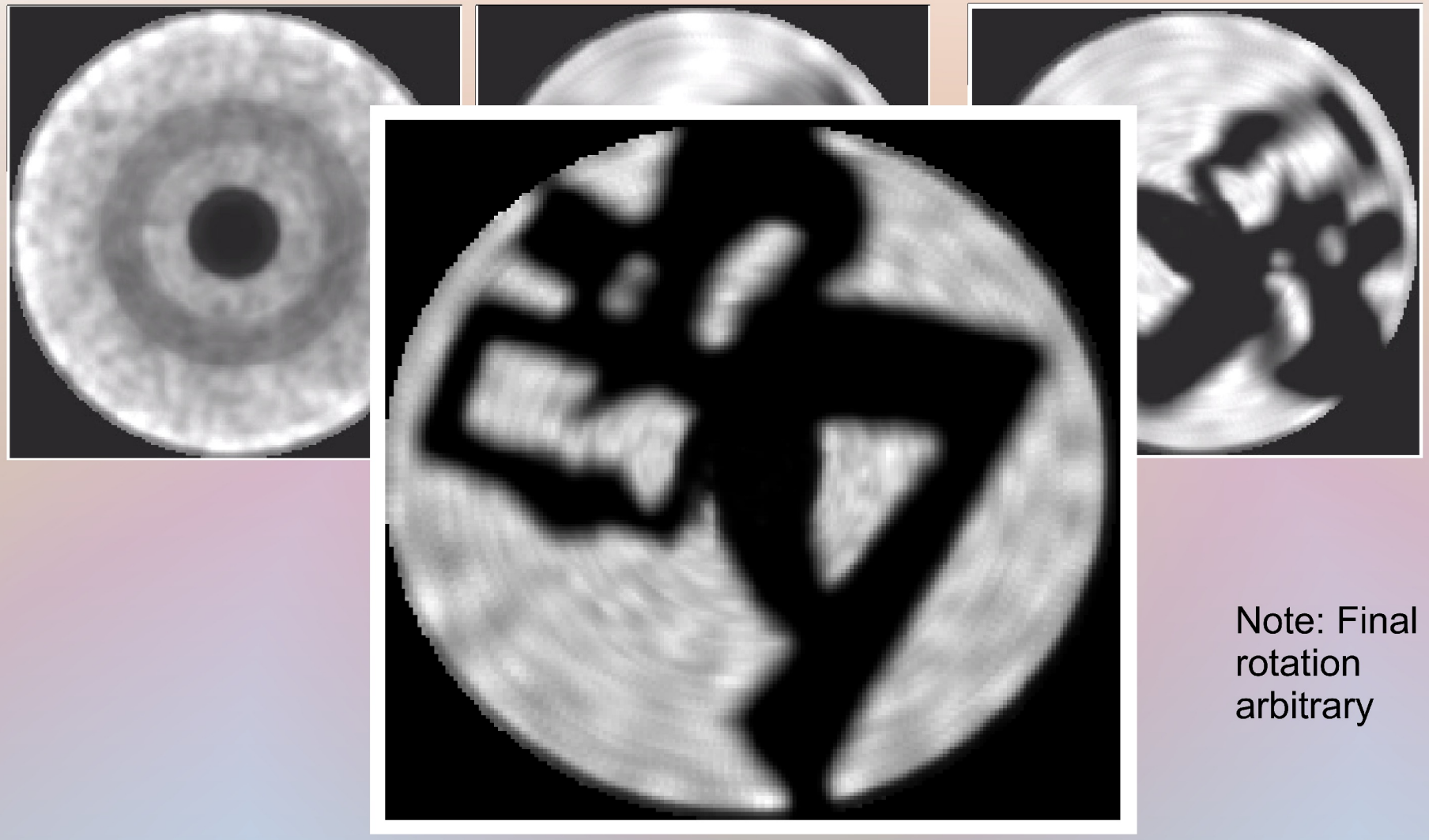
t = pixel index, d = data frame, k = pixel value for data frame, λ = model value



2.5 photons/frame

H. T. Philipp, K. Ayyer, M. W. Tate, V. Elser, and S. M. Gruner, "Solving structure with sparse, randomly-oriented x-ray data," Opt. Express 20, 13129-13137 (2012).

Cornell PAD Development



2.5 photons/frame

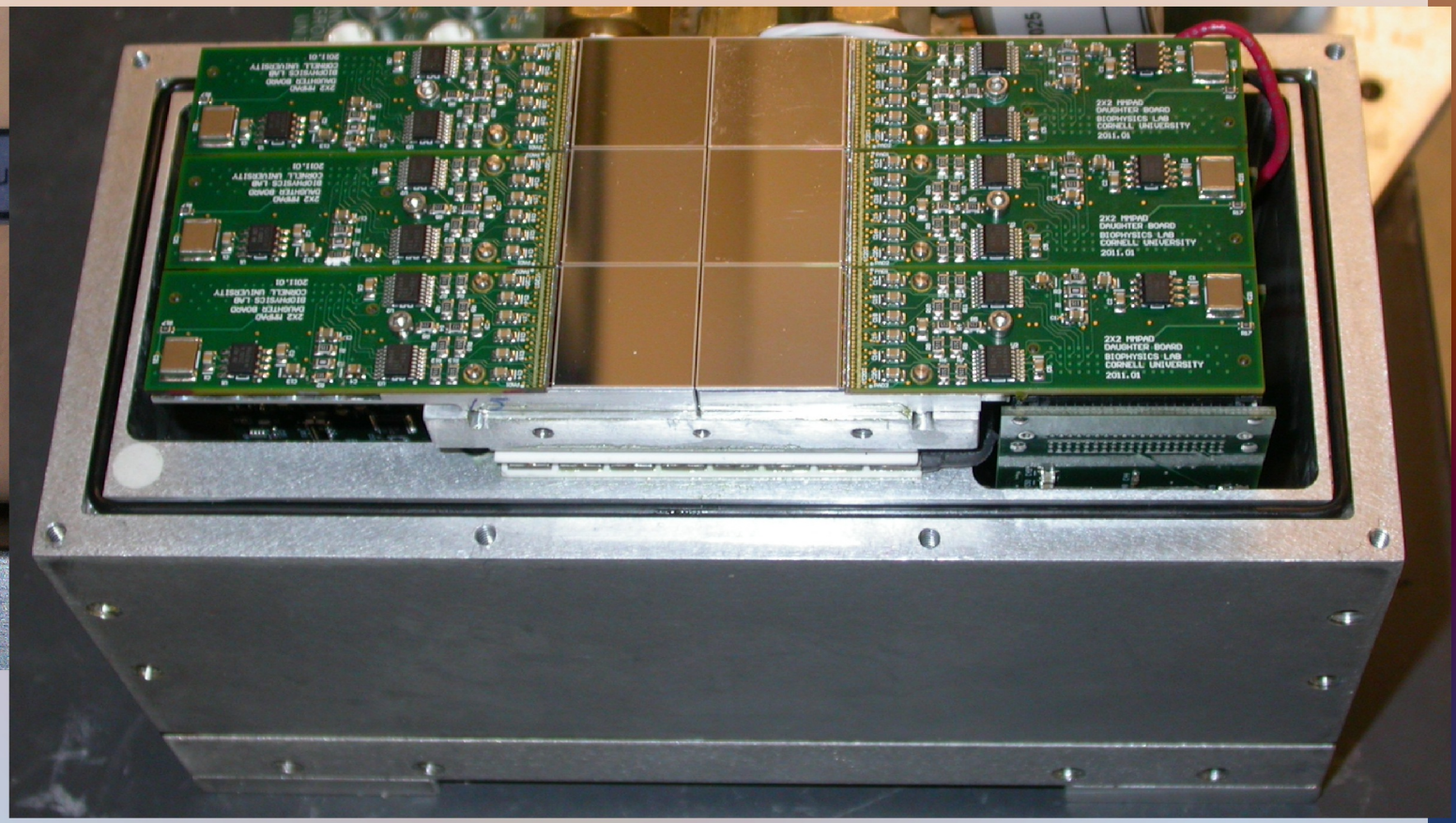
Note: Final rotation arbitrary

H. T. Philipp, K. Ayyer, M. W. Tate, V. Elser, and S. M. Gruner, "Solving structure with sparse, randomly-oriented x-ray data," Opt. Express 20, 13129-13137 (2012).

Attempting 3D

- Lower contrast, 3D object should work in principle.

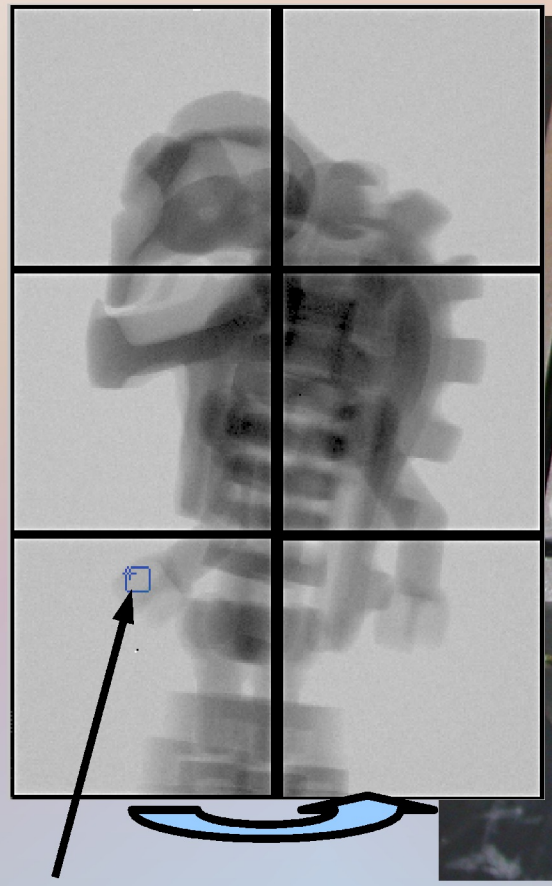
Different Object

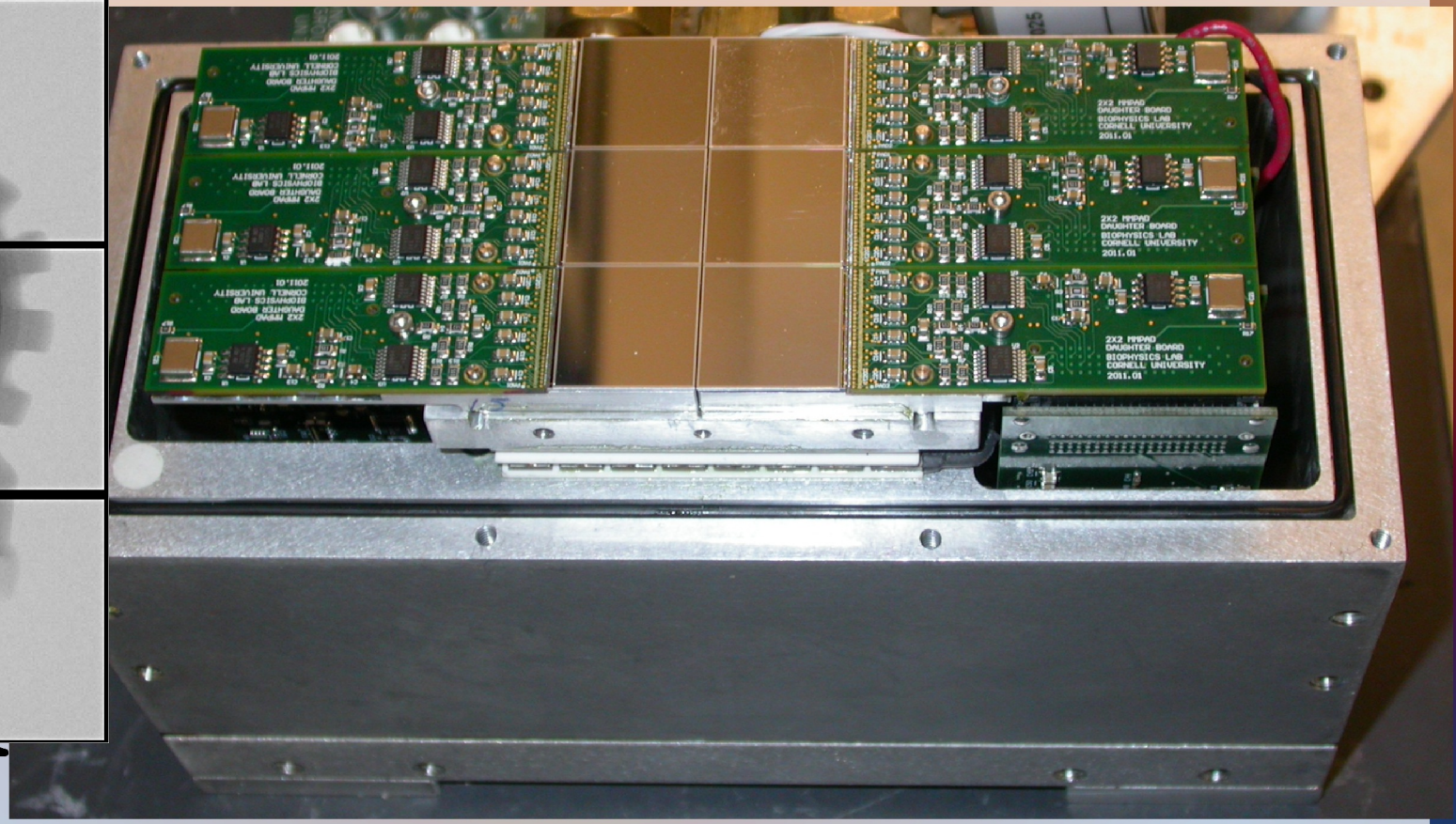


MMPAD: see Posters: WE-F-P-15, WE-F-P-21

Attempting 3D

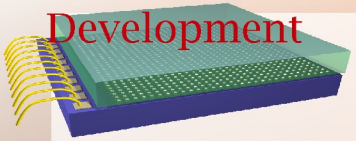
- Low contrast, 3D object should work in principle.



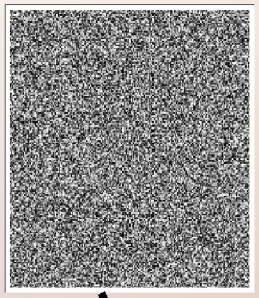


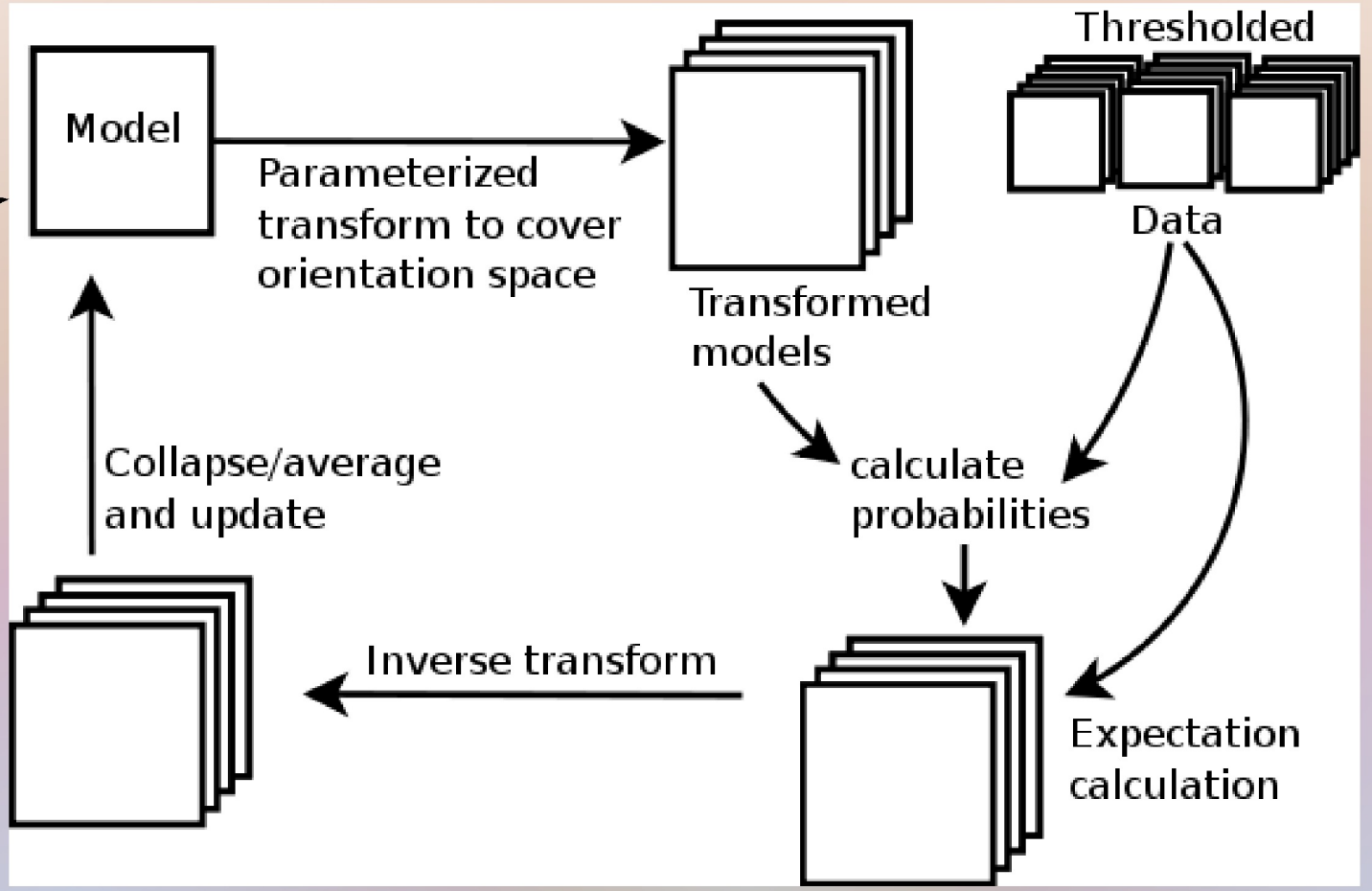
Low contrast: 10-20% attenuation

MMPAD Detector (see poster)

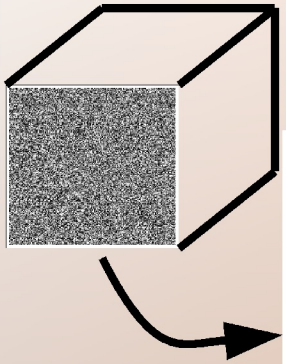


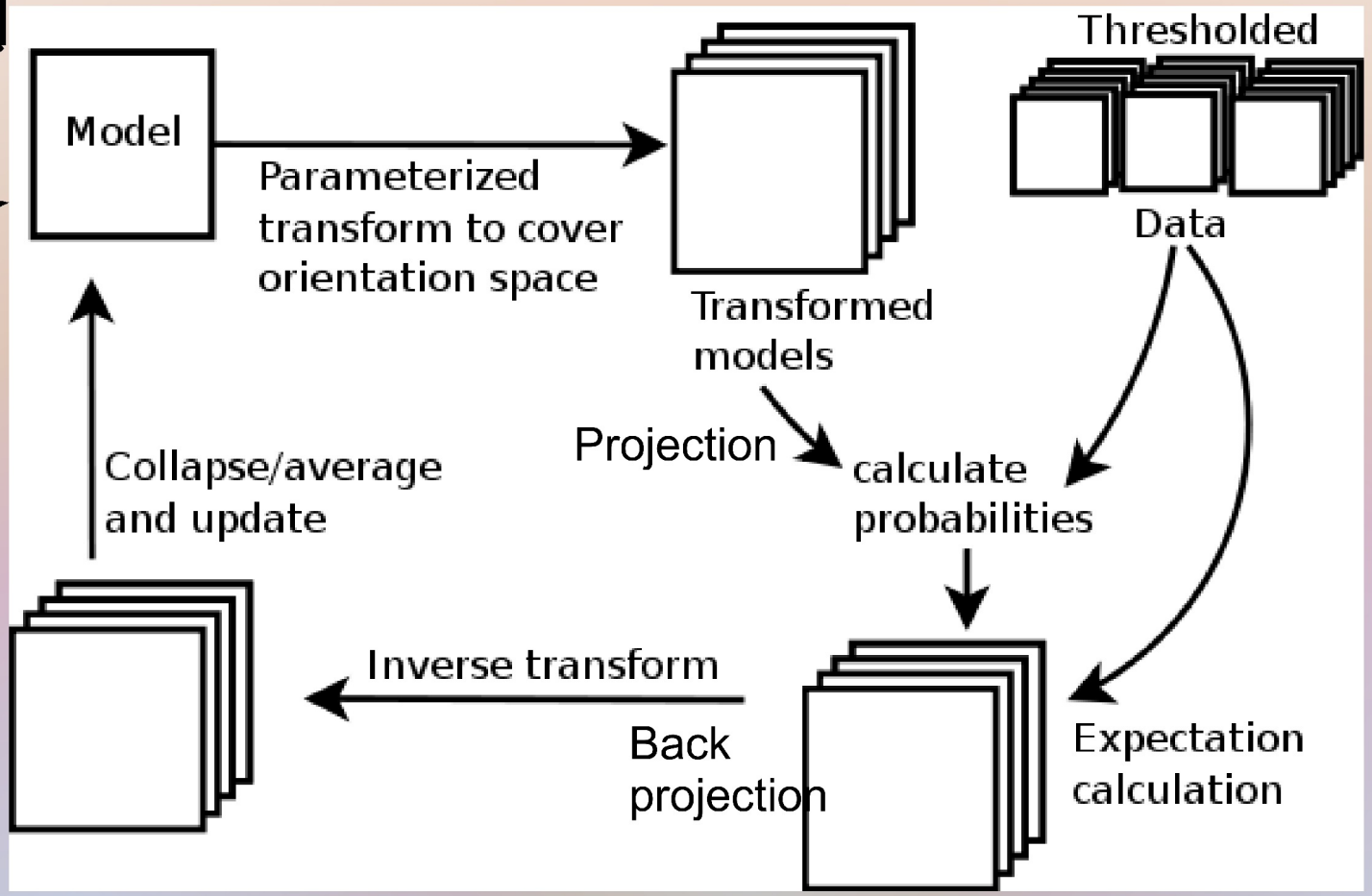
Algorithm almost the same



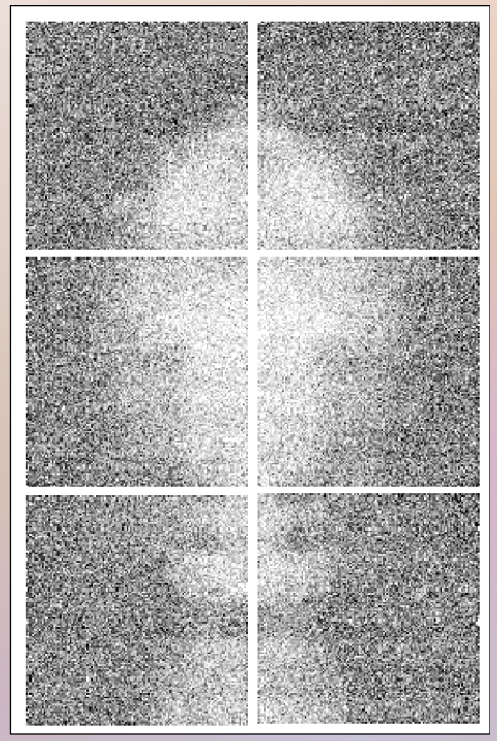


Algorithm almost the same

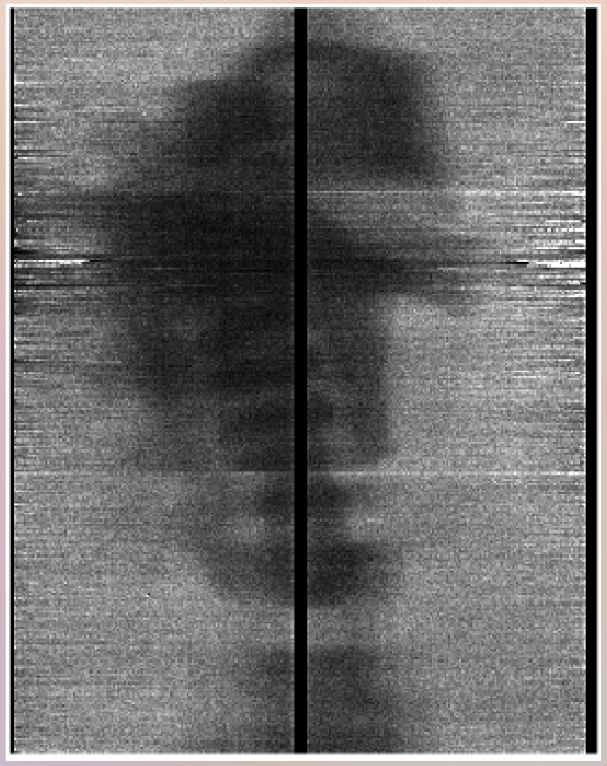




Very Preliminary Results



5000 added frames

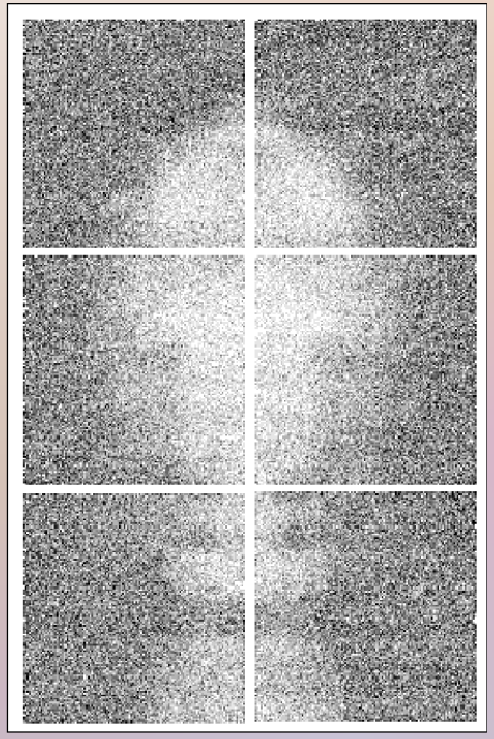


First recovery (projection of model)
- inverse grey-scale

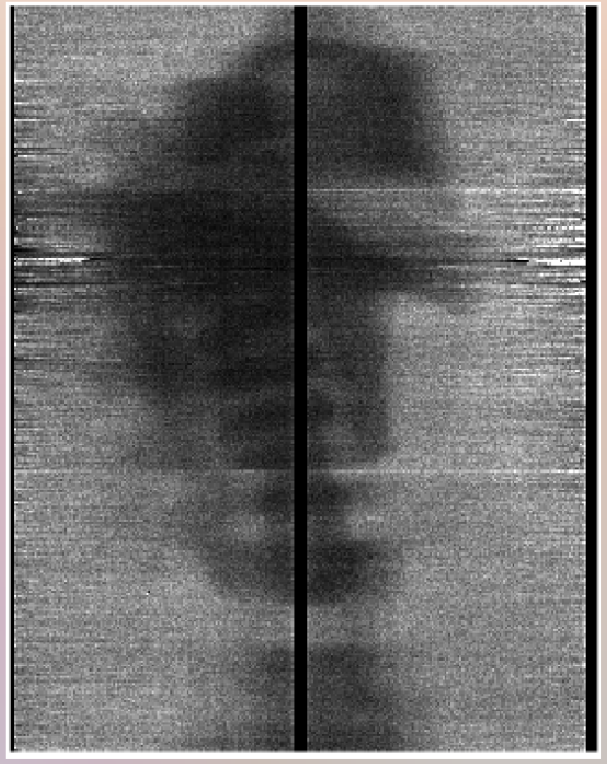
This data set:

- ~ 10^6 frames
- ~ 111 photons/frame
- 300 rotational divisions
- x-rays: 11 to 15 keV
  broad bremsstrahlung
  threshold window

Very Preliminary Results



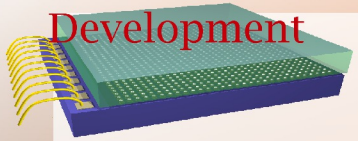
5000 added frames



First recovery (projection of model)
- inverse grey-scale

- Takes long time to reduce

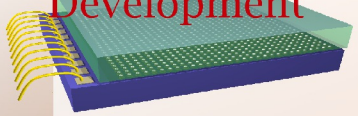
- Classification for first reconstruction ->
  modification of algorithm.



Conclusions

- Must reduce/threshold integrating detector data when extracting information from many frames.
- Expectation maximization algorithms can work.

- WHAT NEXT:
  - instead of playing with LEGOs and lead cutouts to prove principle → using more interesting samples.
- Other:
  - Millions of frames of data can be cumbersome – smarter detector?



Thanks

- Kartik Ayyer, Mark Tate, Veit Elser, Sol Gruner.

- People currently working on detectors:
  - Kate Green, Marianne Hromalik, Prafull Purohit.
  - Darol Chamberlain, Charleie Strohman,
- Some past members:
  - Lucas Koerner, Dan Schuette, Alper Ercan.