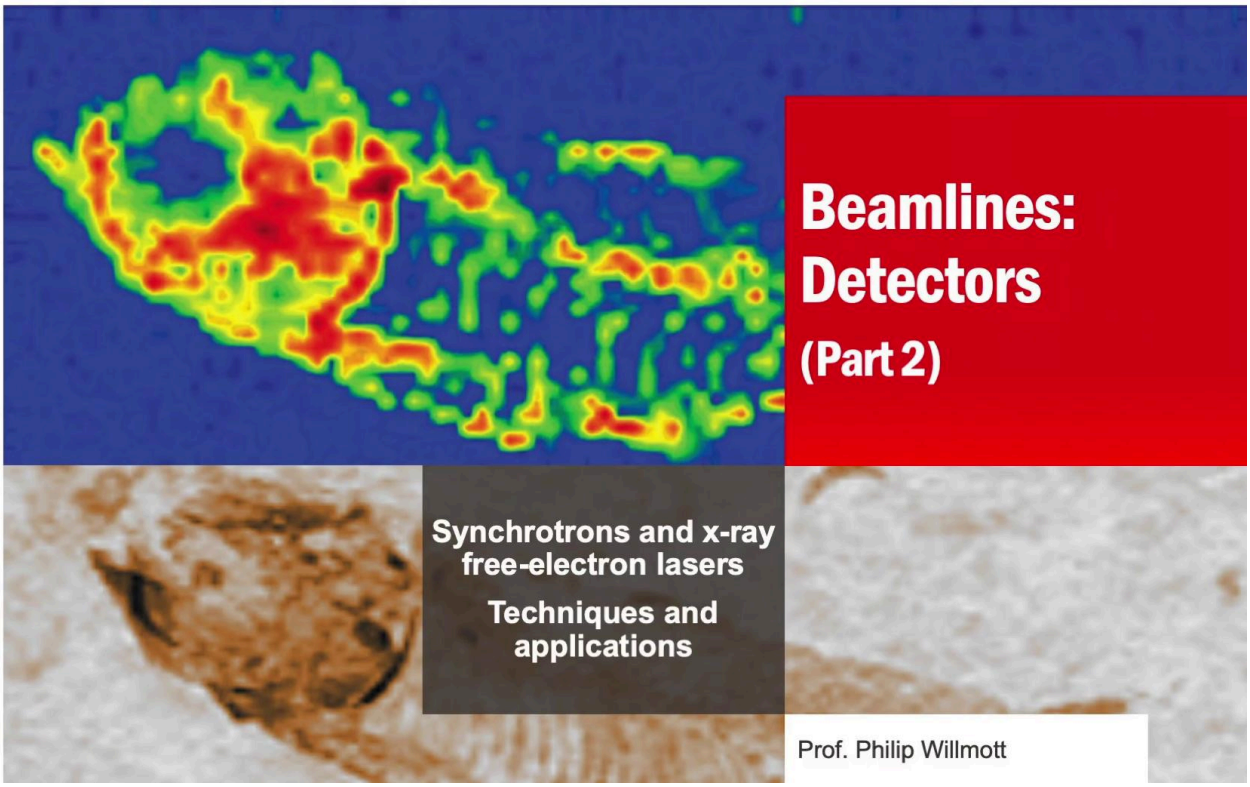
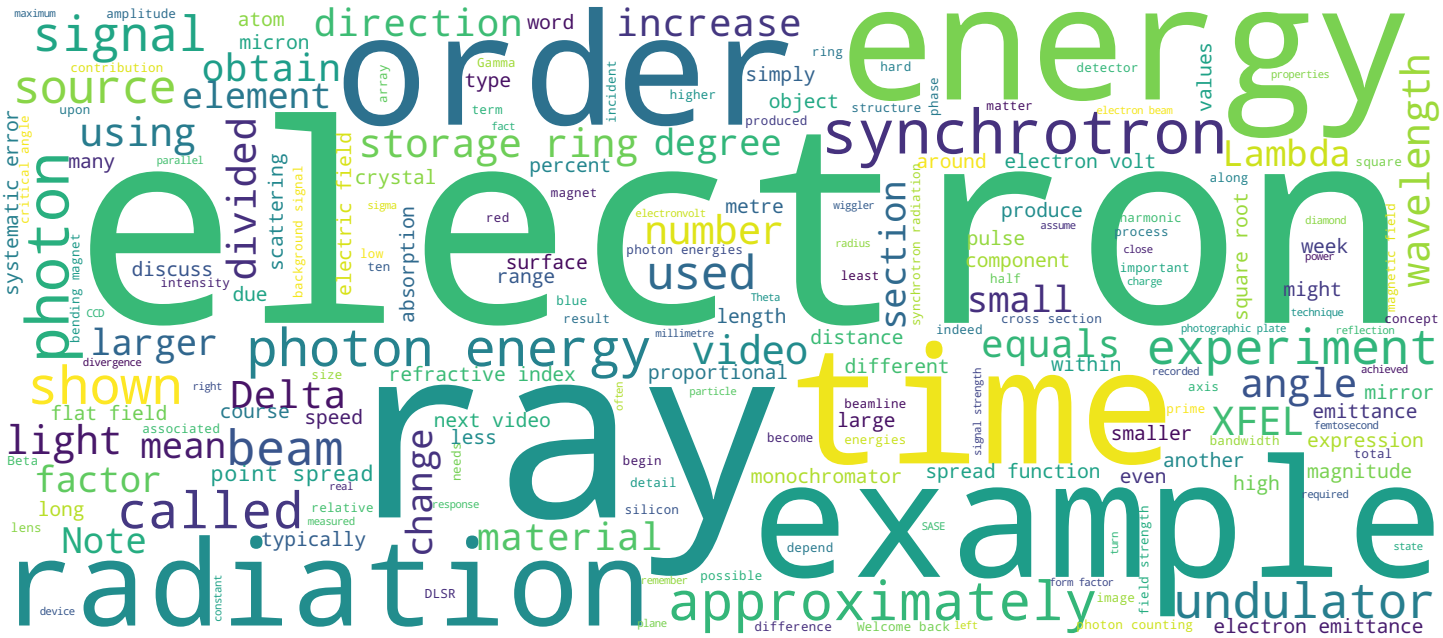




Search MOOC

Video

Contents and objectives of this video

- X-ray detectors
  - What they should do
  - Signal-to-noise ratios
  - Systematic errors
    - Flat field
    - Point-spread function

Hi and welcome back. In this video, we will first consider what the synchrotron experimentalist wants from an x-ray detector and what should be avoided. Next, we look at signal-to-noise ratios, including extracting a signal from a background, and what level of accuracy is really required. We finish this video by reviewing so-called flat fields and point-spread functions.

Notes

Summary

0m 04s

X-ray detectors – what they should do

- Convert x-rays to produce
  - Chemical reactions (e.g., photographic plate)
  - Visible light (phosphor-, scintillator screens)
  - Electrons (CCDs, hybrid pixel detectors)
- Desired properties
  - Spatial distribution of signal resolved
  - High sensitivity
  - Signal strength ∝ electron/x-ray intensity
  - Signal strength ∝ electron/x-ray energy
  - Record weak and strong signal simultaneously
    - High “dynamic range”
  - High frame rate
  - Artefacts minimized

An x-ray detector should convert x-ray photons to produce a signal that is proportional to the x-ray photon signal. Depending on the type of detector, the signal may register a single digital event every time it detects a photon, with little distinction of the photon energy, at least above some threshold value, or otherwise, it might produce an output that varies in a predictable manner with the photon energy. Now, in the early days of x-ray science, the main method used to detect x-rays was with photographic plates. These produce signals that are highly non-linear, they easily saturate, and are thus very difficult to interpret. Despite this, many early breakthroughs in structural biology were enabled through recording diffraction patterns using photographic plates. The person who, more than anyone else, did pioneering studies to quantify diffraction data intensities recorded on photographic plates was Dorothy Crowfoot Hodgkin, who would herself win the Nobel Prize in Chemistry in 1964 for her determination of the structure of penicillin through x-ray diffraction. Anyway, by converting x-rays to light in the visible or near-visible regime, they become more amenable to detection, due to the very much higher interaction strength of these lower energy photons with matter.

Notes

Summary

0m 33s

X-ray detectors – what they should do

- Convert x-rays to produce
  - Chemical reactions (e.g., photographic plate)
  - Visible light (phosphor-, scintillator screens)
  - Electrons (CCDs, hybrid pixel detectors)
- Desired properties
  - Spatial distribution of signal resolved
  - High sensitivity
  - Signal strength ∝ electron/x-ray intensity
  - Signal strength ∝ electron/x-ray energy
  - Record weak and strong signal simultaneously
    - High “dynamic range”
  - High frame rate
  - Artefacts minimized

This process is achieved in phosphor and scintillator screens, briefly described in the next video. Now, most modern detectors record the electrons produced by absorption of the x-rays, such as in CCDs and hybrid pixel detectors, also covered later in this second section of week six.

Notes

Summary

2m 17s

Quantifying signal-to-noise ratio (SNR)

- $I = S + B$
- $\Delta I = (S + B)^{1/2}$
- $\Delta S = S^{1/2}$
- $\Delta B = B^{1/2}$
- $(S + B)^{1/2} \geq S$?
  - Signal lost in background noise!
  - B and S increase linearly with exposure time
- Possible solutions:
  - Reduce B if possible (i.e., if not sample-related)
  - Increase exposure time until $(S + B)^{1/2} < S$

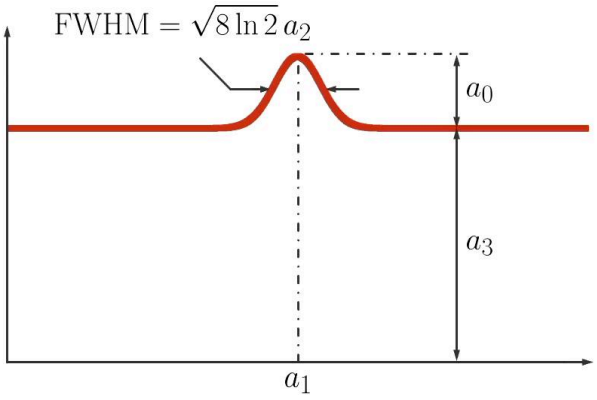
So how long would one have to record a signal to obtain a given accuracy? Clearly, recording a weak signal will take longer if it sits on a significant background signal. A background signal may be real, such as in diffuse scattering, or an artefact, such as scattering off experimental equipment, such as a vacuum vessel x-ray window, if, for example, the sample needs to be protected from ambient air conditions. Okay, so let's assume the total signal, I, equals S, the desired signal, plus B, a background signal. The standard deviation errors of I, S, and B are equal to the square root of those signals, at least for signal strengths that allow the Poisson distribution to be approximated by a Gaussian normal distribution. So if the error in I, in other words, the square root of S plus B, is approximately equal to or larger than the signal strength, S, the latter will be lost in the background noise. Both B and S increase linearly with exposure time. If the background signal is unwanted and not a real part of the system under investigation, it makes sense to try to minimise this as much as possible in advance. Otherwise, one needs to increase the exposure time until the signal strength dominates over the total noise.

Notes

Summary

2m 44s

Quantifying signal-to-noise ratio (SNR)



$$I = S + B = a_0 \exp[-(x - a_1)^2 / 2a_2^2] + a_3$$

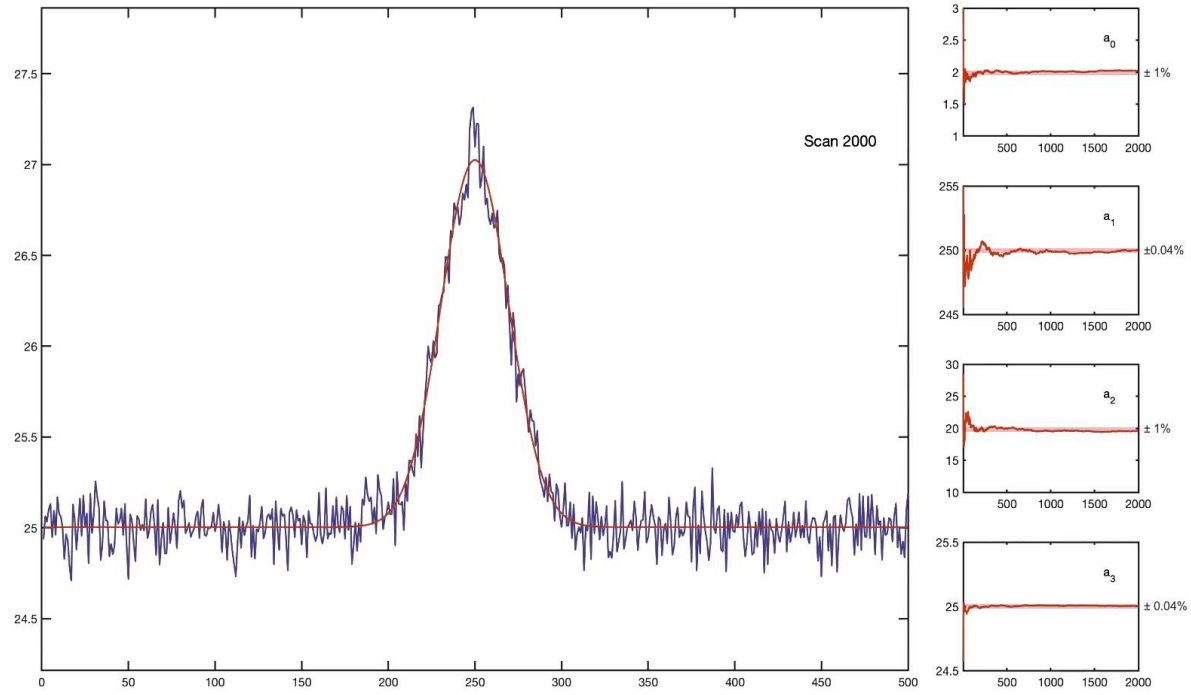
Right. Let's look at an example of a weak Gaussian peak sitting on top of a constant background, which we model with a signal being equal to a0 exponent to the minus x, minus a1 squared, divided by a2 squared, and the background equal to a constant, a3.

Notes

Summary

4m 24s

Quantifying signal-to-noise ratio (SNR)



We look now at a simulation in which a signal with an amplitude of two counts per scan, sitting on a background of 25 counts per scan. We accumulate exposures, normalising each time, by dividing the output by the number of recorded exposures, in order to more easily track the fitting parameters, a0 through a3. Each new accumulated signal is then fit to a Gaussian on a constant background. Okay, so let's start. After a few oscillations that decay in the first few hundred scans, the values for the four fitting parameters settle down to values that don't change by more than a percent, or substantially less, in the case of the background intensity and the central position of the Gaussian peak. Depending on what you want to extract from your data, and to which accuracy you need to do this, you can often stop an experiment long before it loses all of its noise, or most of its noise.

Notes

Summary

4m 53s

SNR – advice

- Take time at start of experiment to implement measures to avoid/minimize unwanted signal (e.g. large background)
- Understand systematic errors
- Record only as long as you need to get data with required accuracy (if known)
  - Increasing S/N ratio by factor X costs X^2 times the recording time
- Overhead time (t_{oh})?
  - e.g. moving motors, transferring data to disc, …
  - Minimize this if possible
  - If $t_{rec} \ll t_{oh}$, then relax above criteria

So what general advice should be heeded when preparing an experiment or a given scan? First, time taken before the experiment to avoid or minimise unwanted signal and identify their origin can often be more than recouped in the experiment itself by having a cleaner signal. So it's worth investing time to prepare your experiment as best you can. Secondly, understanding the source of systematic errors is also very important. Next, record only as long as you need to. Obtain the required accuracy. Polishing by a factor of x beyond that which is necessary will cost you x squared in effort or time. Lastly, one should not neglect overhead times needed, for example, to move motors or transfer data to disc. If it turns out that the overhead time is substantially larger than the recording time, then the criteria to record only the minimum to obtain the required accuracy can be somewhat relaxed, if you want to have nice-looking data.

Notes

Summary

6m 00s

Systematic errors

- Systematic error: mean of many measurements not a good estimate of true value
- Examples
  - Incorrect energy calibration
  - Partial or uneven occlusion of signal
  - Flat field
  - Point-spread function (imaging)
  - Timing inaccuracies
  - Sample degradation (radiation damage)
  - Pile-up (photon-counting)
  - Saturation
  - Blooming (CCDs)
  - …

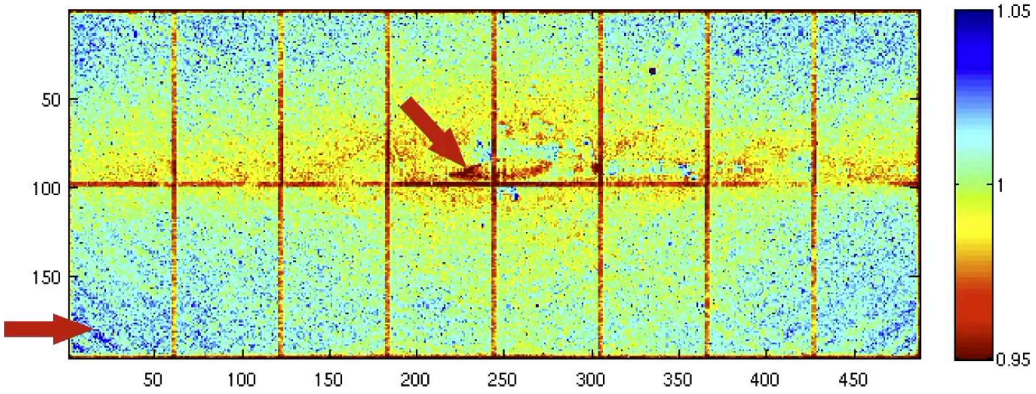
We just mentioned systematic errors, but what defines a systematic error? In general terms, one can state that a systematic error occurs if the mean of many measurements of a signal is not a good estimate of its true value. Examples of sources of systematic errors include incorrect photon energy calibration, partial or uneven occlusion of a signal, such as when you use a filter of a nominal known attenuation, but which is cracked or partly shattered. I speak from personal experience here. Neglecting flat-field corrections or using the wrong flat-field correction is another example. We discuss what a flat field is in just a moment, along with the concept of the point-spread function. Timing inaccuracies, for example, sluggishness in opening or shutting of an exposure shutter, sample degradation, or radiation damage, are all further examples of systematic errors. Photon pile-up in photon-counting detectors is another one. Saturation, blooming. The list goes on, and on, and on. I will touch on these last three mentioned phenomena of pile-up, blooming, and saturation in the next videos.

Notes

Summary

7m 13s

Flat field



- False-colour image of a flat-field correction array in a photon-counting detector (Pilatus 100k, 2nd generation)
  - Colour bar displays the corresponding flat-field correction factors (note scale)
  - Red pixels are more sensitive than the average – their values need to be decreased
  - Blue pixels are less sensitive and need to be amplified

Image courtesy of C.M. Schlepütz, Paul Scherrer Institut

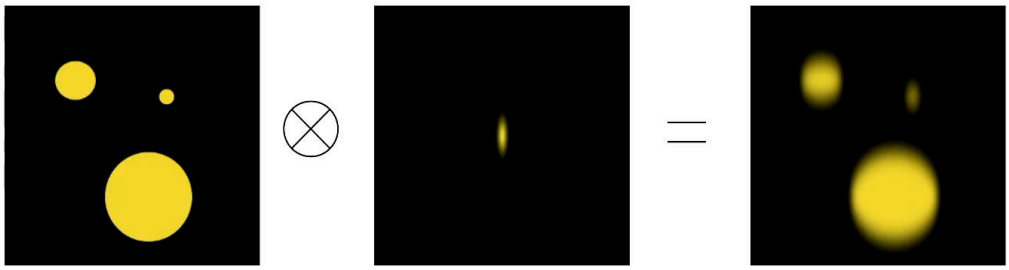
Now, flat fields are arrays that reflect the variation of the response of a detector across its sensitive area. Shown here is an early flat field of a second generation Pilatus 100k hybrid pixel detector. This was recorded in around 2007, I believe. Note that the range of colours from dark red, through green to dark blue, only spans plus or minus five percent. Having a low value, red on orange, means that the pixel is more sensitive. The blue and cyan pixels are less sensitive. The blocks delineated by the red lines show the edges of the 16 photon sensitive elements that are bump bonded onto the larger silicon readout chip. This itself has curious arc features, such as highlighted here, which reveal the action of the diamond saw which was used to slice the chip from the original boule of silicon. A more prominent feature is the red blob close to the centre, where the filtered direct beam and small diffraction features would typically be detected. The occasional over-exposure, caused by forgetting to insert an appropriate filter, resulted, after approximately two years, in the formation of this anomalously sensitive patch.

Notes

Summary

8m 33s

Point-spread function



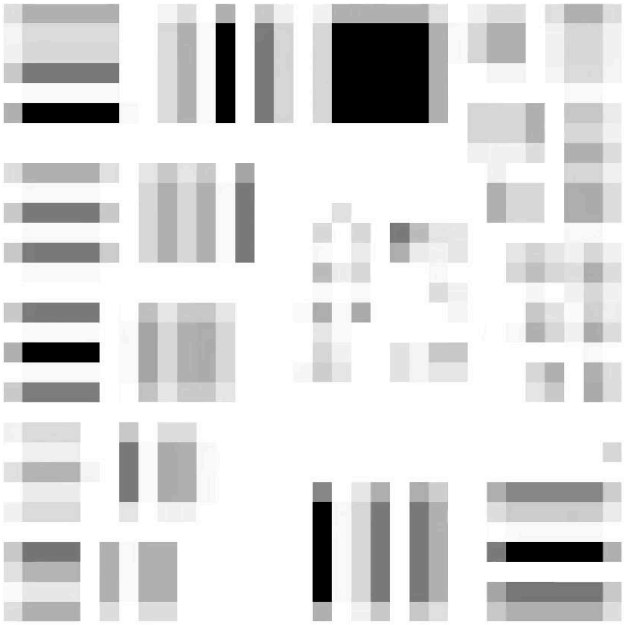
The point-spread function describes the response of an imaging system to a point source or point object. So for example, a pixelated detector cannot have a smaller point-spread function than the detector's pixel size. If the PSF, point-spread functions, across all elements of a detector are identical, then the image of an object is simply the convolution of that object with the point-spread function.

Notes

Summary

10m 02s

Point-spread function



1600 x 1600 pixels

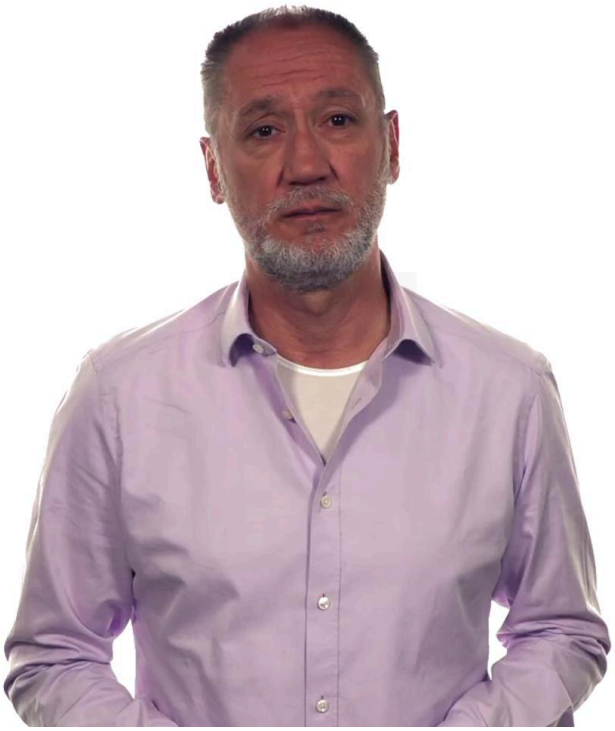
In this animation, we see how an optics resolution image with the size of 1600 by 1600 pixels becomes increasingly blurred if it is raster scanned with a square-point detector of increasing size from one by one to 50 by 50 pixels. Note that, if instead, an area detector is used with pixel sizes equal to 50 by 50 of the image pixels, the quality is even poorer.

Notes

Summary

10m 33s

In the next video...



In the next video, we consider the different approaches of either photon counting or integrating detector types, and take a closer look at hybrid photon-counting detectors.

Notes

Summary

11m 07s