Detector Pool Guide to the Bruker SMART 6500

By Tim Madden
Bruker_6500_Users_Guide_V3.doc

REVISION HISTORY:
3/2005 Original
9/ 2005 merged in the "how it works section" (steve)

INTRODUCTION:
The detector pool and XOR sector 1 now share a Bruker Smart 6500 x-ray ccd detector. Typically XOR will have some first opportunities to reserve it before general reservations start, but otherwise it is a normal "Pool" detector.

We are working to make the detector robust (making a cart to move it around), and documented (software etc). This User Guide is the main document on the detector.

CONTACTS AT BRUKER:
We have a service contract.
Eric Boyce- Tech support guy.
1-800-234-XRAY
Eric Amble- another support guy. He set up our visit from Bruker service.
1-800-234-XRAY
Gary Ganly- Field Service Engineer- He is coming to ANL Wednesday, 10/20/04
Cell Phone: 630 347-6012.
Bruker is at **www.bruker-axs.de**

INVENTORY PARTS OF THE BRUKER 6500 SYSTEM:

DP00165	Bruker detector head CCD camera
DP00166	Bruker 6500 CEU
DP00167	Bruker 6500 Crate
DP00168	Bruker 6500 power supply module
DP00169	Bruker 6500 Chiller

More items to be added, list not complete

SPECIFICATIONS OF DETECTOR:
These will be further discussed below.

Readout time about 3 sec (full 2K x 2K image)
Dynamic Range TBD

CCD Gain: 5e-/ADU.

CCD Read noise: 70e-
CCD Dark Current: 4e-/pixel-s 2K mode
15 e-/pixel-s 1K mode

Pixel Size: This will be discussed in detail below. At the x-ray imaging active area:

0.163mm(1K mode corrected)
0.159 mm (1K uncorrected)

0.078mm uncorrected 2K
0.081mm corrected 2K

Pixel size measured to be 0.126mm in 1K mode when software has unknown setting.(Using distance factor)

USING THE DETECTOR – HOW IT WORKS.

The detector system is a large white box on wheels containing several components, a chiller, PC, and detector head. See attached picture.

What each box is:
The Smart 6500 system includes the following components:

Detector Head- The detector head has a front-illuminated Fairchild CCD485 glued to a taper with optical epoxy. The head has electronic preamplifiers to send an analog image signal to the CEU. A cooling probe can cool the detector to -95C which will break the detector. Thermal resistors heat the detector to regulate its temperature to -45C. The CEU must be ON if the chiller is on, to provide regulation. The detector head contains a ROM which is the CCD timing and software for the CEU to run. The CEU downloads from this ROM on startup. Several cables and a large hose connect to the head.

CEU- A rack mount unit with a square switch and LCD on the front. It looks a little like a PC, but there is no hard drive in it. The CEU is the power supply and timing generator for the detector head. All DC bias voltages and CCD clocks are probably generated here. The ADC converters reside in the CEU to digitize the image data.

Crate- This is a crate of cards looking a bit like a VME crate. It runs on 270V, boots from a floppy, and controls a shutter and goniometer. It has a TTL signal output to the CEU to trigger exposures in the camera. Bruker “requires” the crate to operate the camera. Probably we can work around that.

Power Supply Module- A metal rack mount unit to power the CEU and chiller. It is a box of relays that can turn on and off the CEU and chiller together. If the CEU trips off, the chiller turns off too. The chiller and CEU should be powered from this to avoid ruining the detector by overcooling it. The CEU can be run for 1 hour or so without the chiller, for testing. The chiller should not be run without the CEU.

Chiller- This is a separate unit that pumps propane into the detector through a large black hose. The propane evaporates in the detector head to cool it. The chiller has 2 stages: a Freon compressor cools the propane compressor; no water is used. The On switch is green, and should glow. A Green LED turns ON meaning the propane compressor is on.

Power Strip1: 110V. Power Supply module and PC plugs in here. Fans on system run from this.

Power Strip2:220V. Crate plugs in here.

Turning it on:
Plug in Strip1 into 110V. Plug in 220V Strip2. Turn on strip1, fans should spin. Hit reset on Power Supply Module, CEU and camera should come on. Turn on PC. Make sure crate is plugged in at front of crate. Crate should boot off floppy. Ask Ulrich Lienert about floppy. Don't worry about waiting for anything or order. Just turn on everything. Turn on chiller. Green Led on chiller should light after several minutes.

For testing, the 220V can be left off. The chiller can be left off if the detector runs for less than an hour. Keep track of temperature displayed on CEU to make sure electronics won't fry.

Turning it off:
Do the above in reverse. Order and timing is not too important.

Software Notes:
A Bruker-supplied PC runs Windows 2K, and the Smart software. This software controls the camera and goniometer. X-Ray crystallography can be calculated with Smart. Smart takes care of camera calibrations, corrections, and geometric correction.

It looks like a Windows 95 program (*ie.* DOS with a mouse).

DETECTOR POOL MEASUREMENTS OF BRUKER 6500.

It is desired to have a comparison of the performance between the Mar 165 and the Smart 6500 detector. To this end, dark images were taken on the Bruker detector to determine the read noise and dark current. Also any other artifacts can be seen. These images were taken when the detector was cooled to -50C in 1K mode. These images were taken without dark current correction, without flood correction, and with and without spatial correction. Flood and dark correction would make dark image analysis useless, as the detector performance would be hidden by the calibration files. Although many aspects of the detector performance can be judged from dark images, more accurate data can be obtained using X-Rays to take flood and pinhole images. This should be scheduled during a machine studies period.

Short Exposures

Images of 1s and 0.1s were taken to analyze electronics noise created by the camera. In 1s images (with the detector at -50C, and dark current very small), some images had areas with less signal. This dark area appears in different areas of the images randomly, and sometimes disappears altogether. It could be a differential linearity problem in the ADC, or random noise pickup. In real data, these dark areas were seen at Sector 1. An image with this dark area is shown below. (Fig. 1).

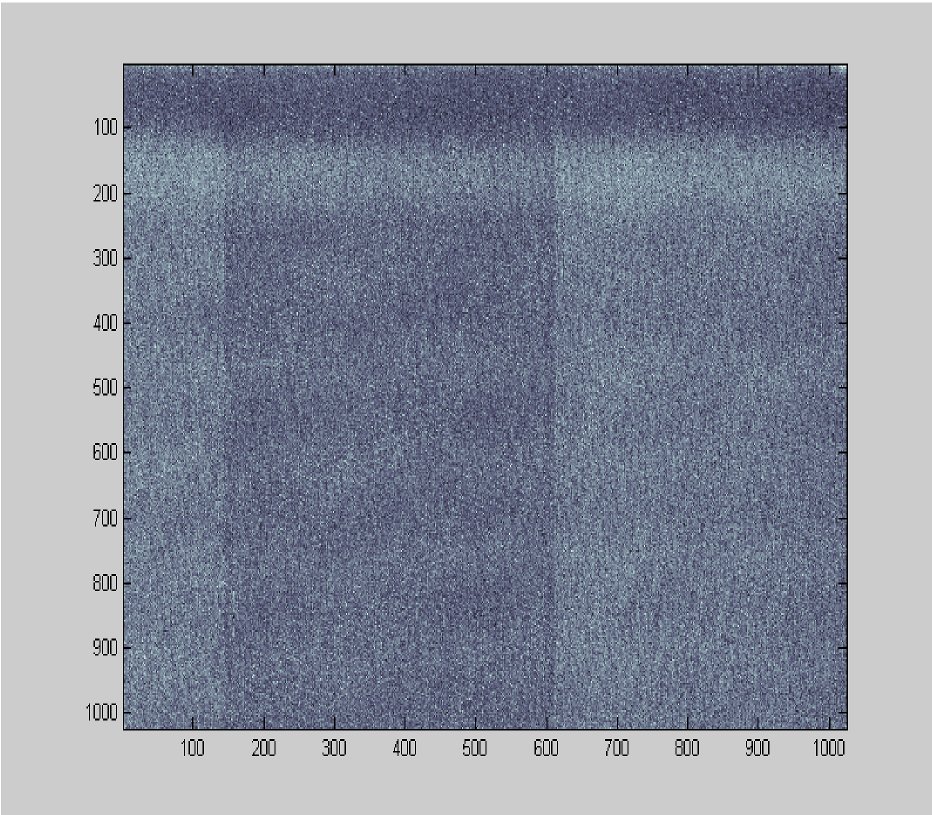


Fig. 1. 1s image, -50C. Note dark area. (Image file: Dc12)

To determine if this dark area is added noise, or less signal, horizontal lines were averaged to tell if the mean signal is less. It was confirmed, in Fig 2, that the dark area is a region of smaller signal.

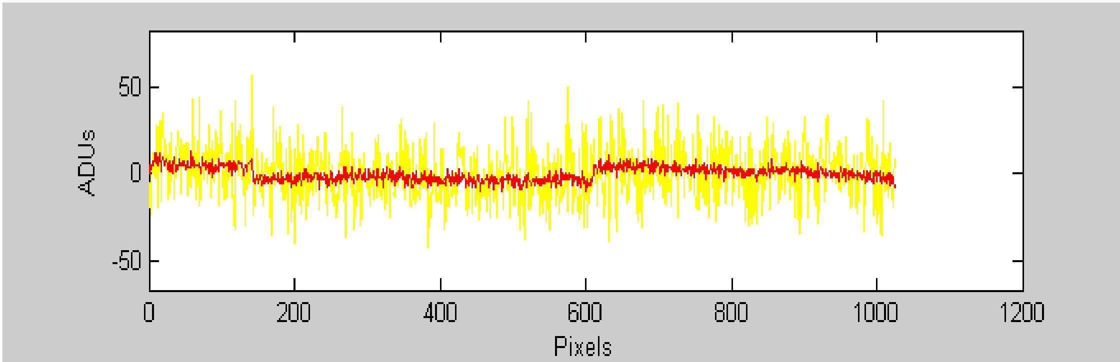


Fig.2. Red line is average (using a Kalman Filter) of 30 horizontal lines in Fig. 1. Yellow is one non-averaged line.

To show how the dark area moves around or disappears, Fig 3 shows another 1s image with no dark area.

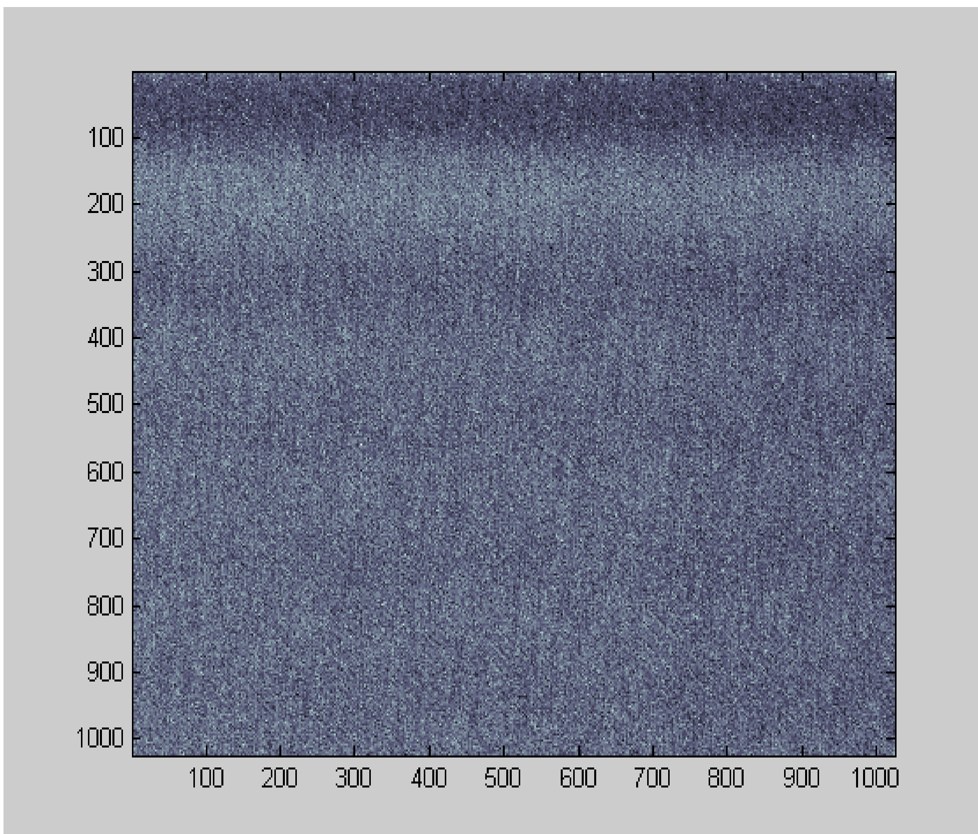


Fig 3. 1s image with no dark area.

FFT Analysis

Looking at the 1s images closely reveals a repeating pattern. To determine if this pattern is real, FFT's of horizontal lines were averaged to find harmonics, denoting real noise signals. The FFT of a 1s image is shown in Fig 4.

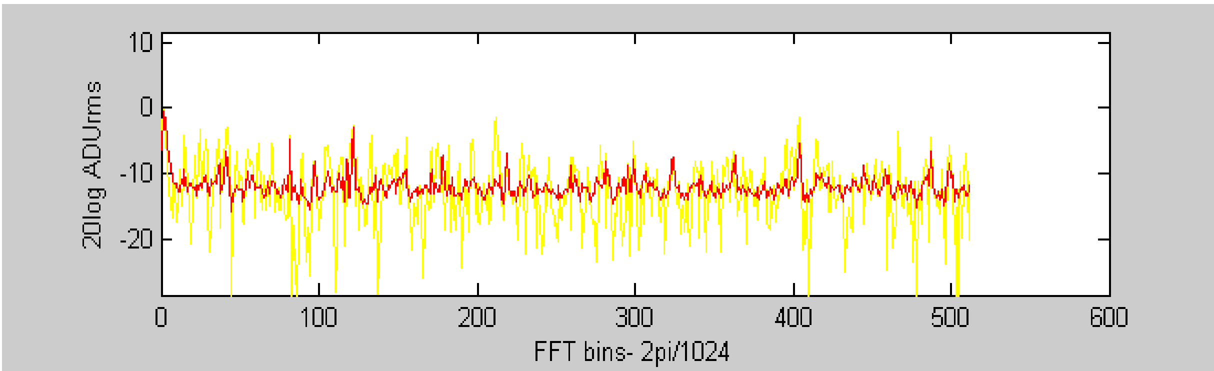


Fig 4. FFT of horizontal lines in 1s dark images. Spurs denote noise pickup, or electronics oscillations. Red is averaged FFT using a Kalman Filter.

These spurs in the FFT's are visible in images of up to 2 minutes integration time. Longer than that, dark current covers up the oscillations.

Taper Image Seen in Dark Current

Long dark current integration times (>60s) reveal that the taper bond to the CCD influences the dark current. This is probably why Bruker does a dark current correction, so the taper is not seen in real data. A 780s exposure (Fig 5) shows the taper, as well as other vertical structures in the dark current.

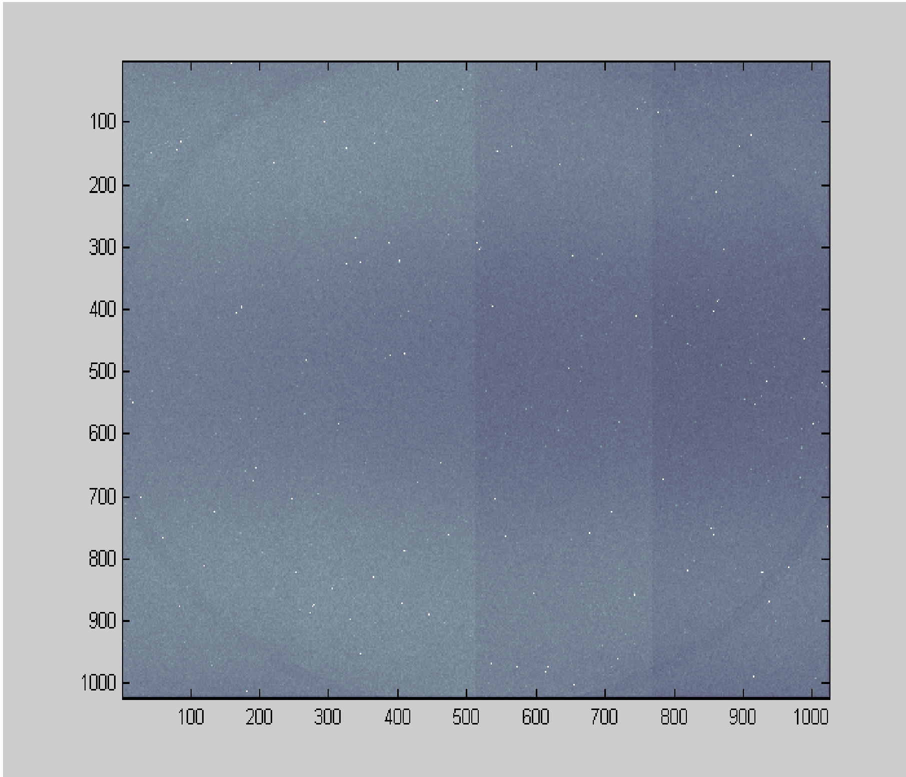


Fig 5. The dark current shows the taper on the CCD. Note the circle. (Dc7810)

Geometric Correction Artifacts

The spline interpolation not surprisingly adds small artifacts to the images. Note in Fig 6, the left side clearly shows each noisy pixel. The right, with spatial correction, side blurs the pixels.

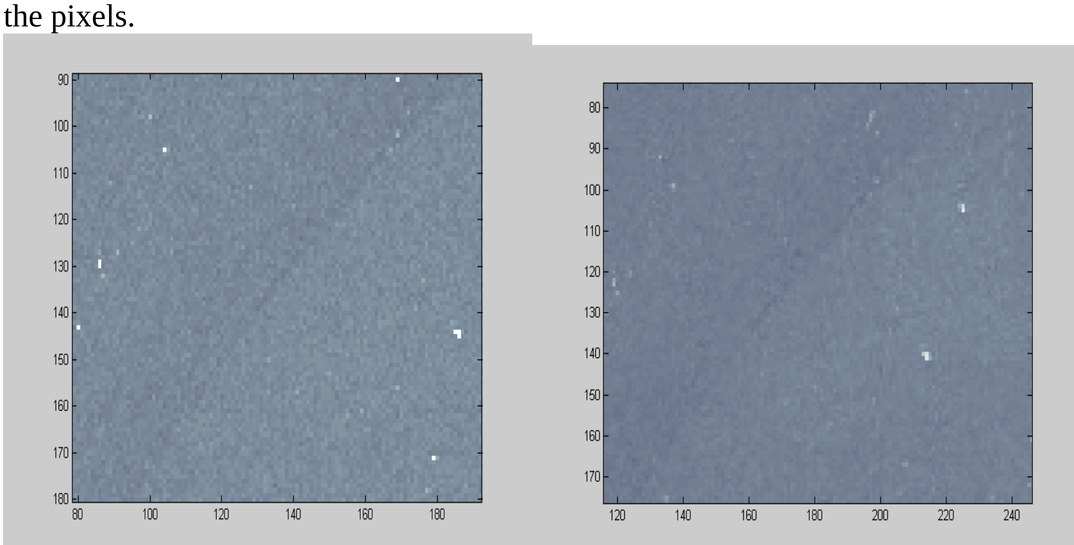


Fig 6. Left side not corrected. Corrected right side shows blurring of the noise.

This blurriness means we really have less than 1K pixel resolution.

Fig 7 shows the whole image of Fig 5 after spatial correction.

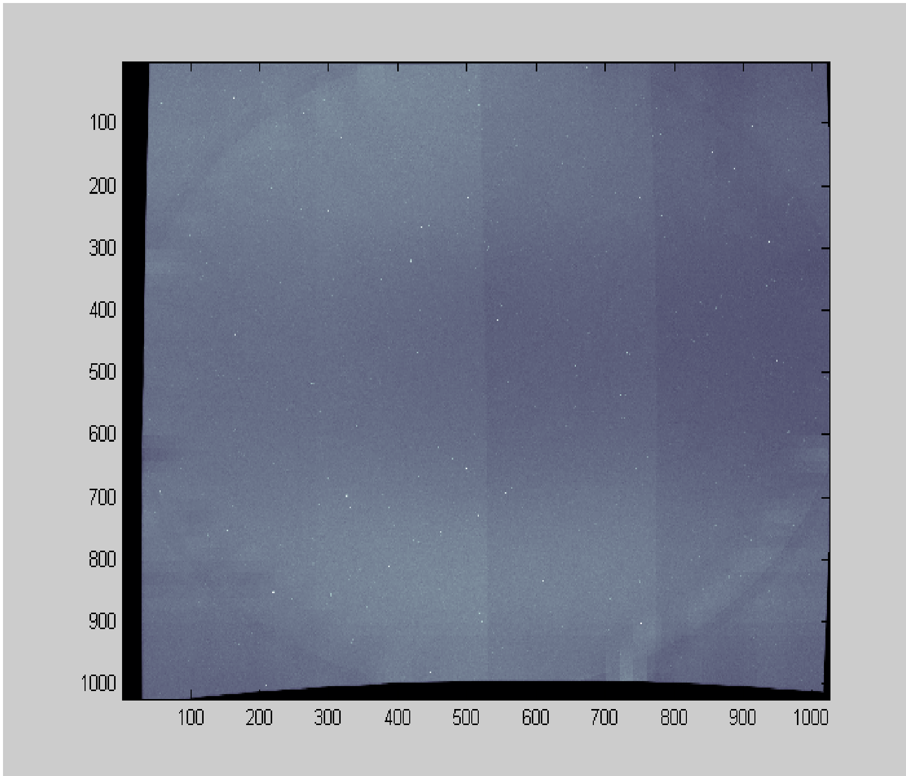


Fig 7. Corrected Fig 5.

Fig. 8 shows the lower right corner of Fig 7. Note the vertical structures added by geometric correction.

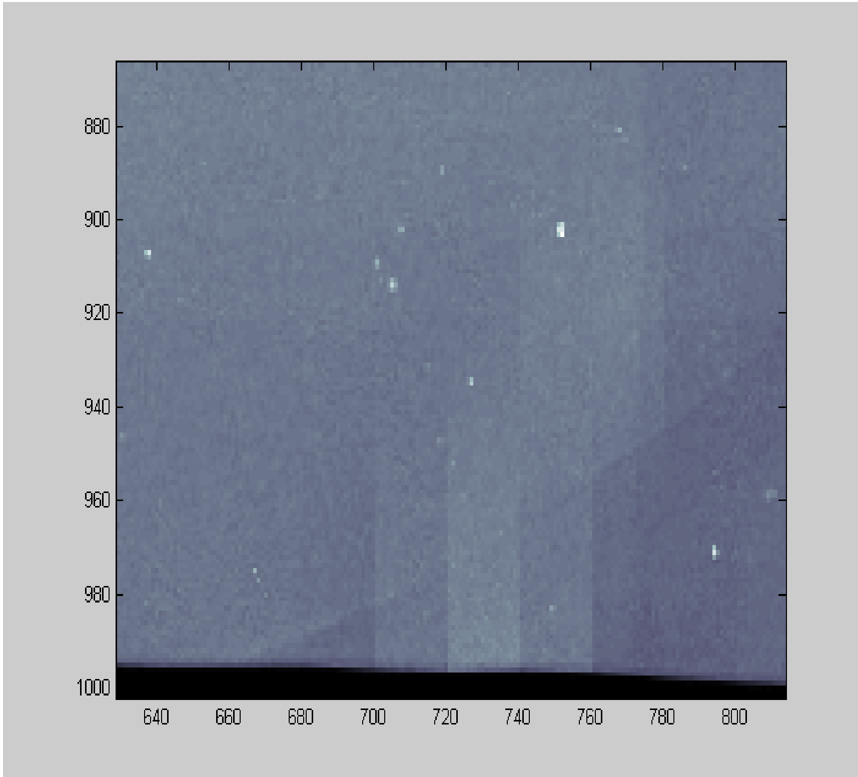


Fig 8. Close up of Fig 7, showing correction-induced artifacts.

Dark/Gain measurements

With the detector cold, at -50C, dark images were taken to determine detector gain as in Janesick, *Scientific Charged-Coupled Devices,* pp 100-110. The idea is that we take images of varying integration times, and plot variance versus mean. The Poisson nature of dark current (and light) gives us the gain of the camera, or a relation of ADU's (Analog-Digital Units, what the image stores) to electrons on the CCD. The quick explanation is that for a Poisson process the variance equals the mean. That is

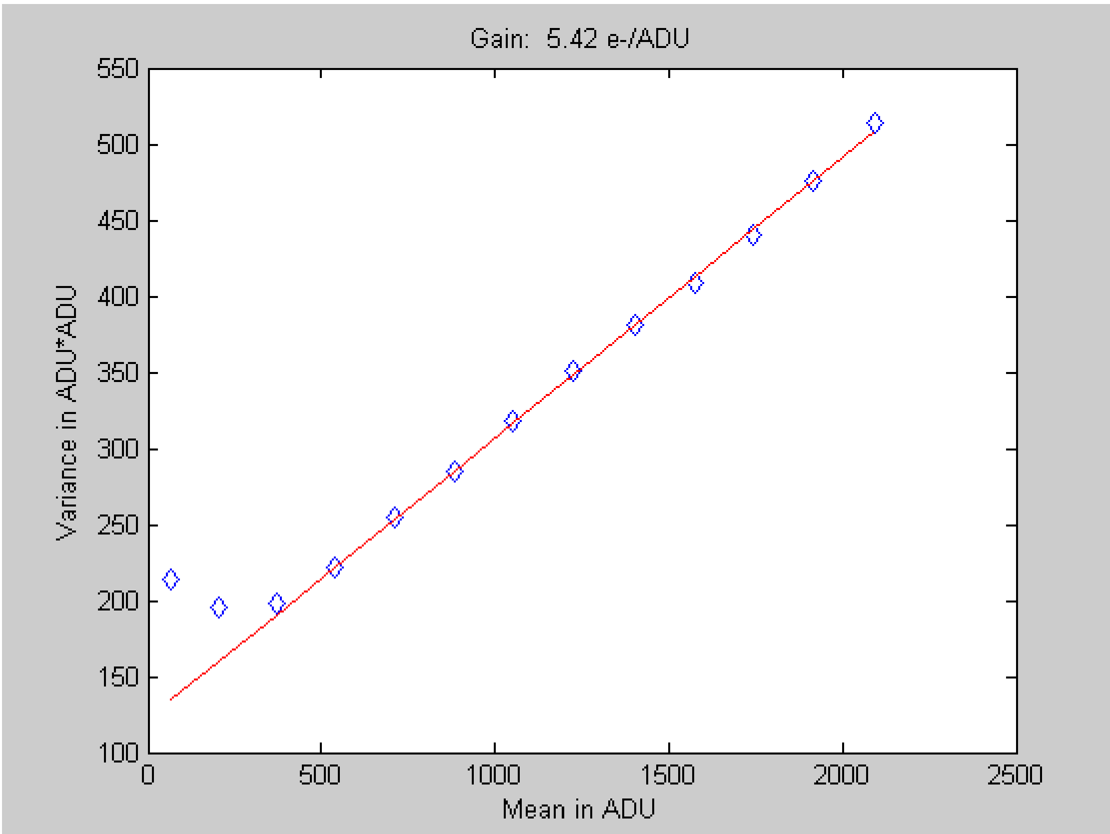
$$\sigma^2 = \mu$$

In the camera, we only measure the signals at the output of the electronics of gain A, in units of ADU/e-. Therefore we see signals with mean and standard deviation of $A\mu$ and $A\sigma$, where μ and σ are in units of e-. The variance of the measured signal is therefore $A^2\sigma^2$ [Appendix]. If we plot mean versus variance the slope,

$$m = \partial(A^2\sigma^2)/\partial(A\mu) = A \;\; \partial\sigma^2/\partial\mu = A \;\; \partial\mu/\partial\mu = A.$$

Therefore, the slope of the line is the conversion factor from electrons to ADUs.

The plot of mean versus variance is shown in Fig. 9.



Fig, 9. Variance versus Mean for dark images. Slope of straight section is the gain of the camera. The rounded section at X=250, is where read noise presides. It is unknown why curve points upward at X=100.

By analyzing this plot, the gain of the detector is about A=.2ADU/e- or 5e-/ADU. Note that the detector was set to a gain setting of 6, in whatever units Bruker uses. Perhaps the Bruker gain setting is in ADU/e-. At low means, where the curve bends upward the read noise dominates, and dark current is negligible. The curve should flatten out. Several data sets had this problem. It could be cause by the dark areas in the images like Fig. 1. Differential linearity problems in the ADC electronics could cause this problem. There is either something wrong with the detector, as Fig. 1 suggests, or something wrong with the data. For a simple approximation, the curve flattens at a variance of about 200ADU*ADU, or about a standard deviation of 14ADUs. This means the read noise is about 70e-, fairly large. Probably the read noise is too high, meaning that the detector broken, or the data is wrong.

To measure dark current, we take a series of dark images at various exposure times. If we plot the exposure time versus the mean signal, the dark current is the slope of the line. A dark current plot is shown in Fig. 10.

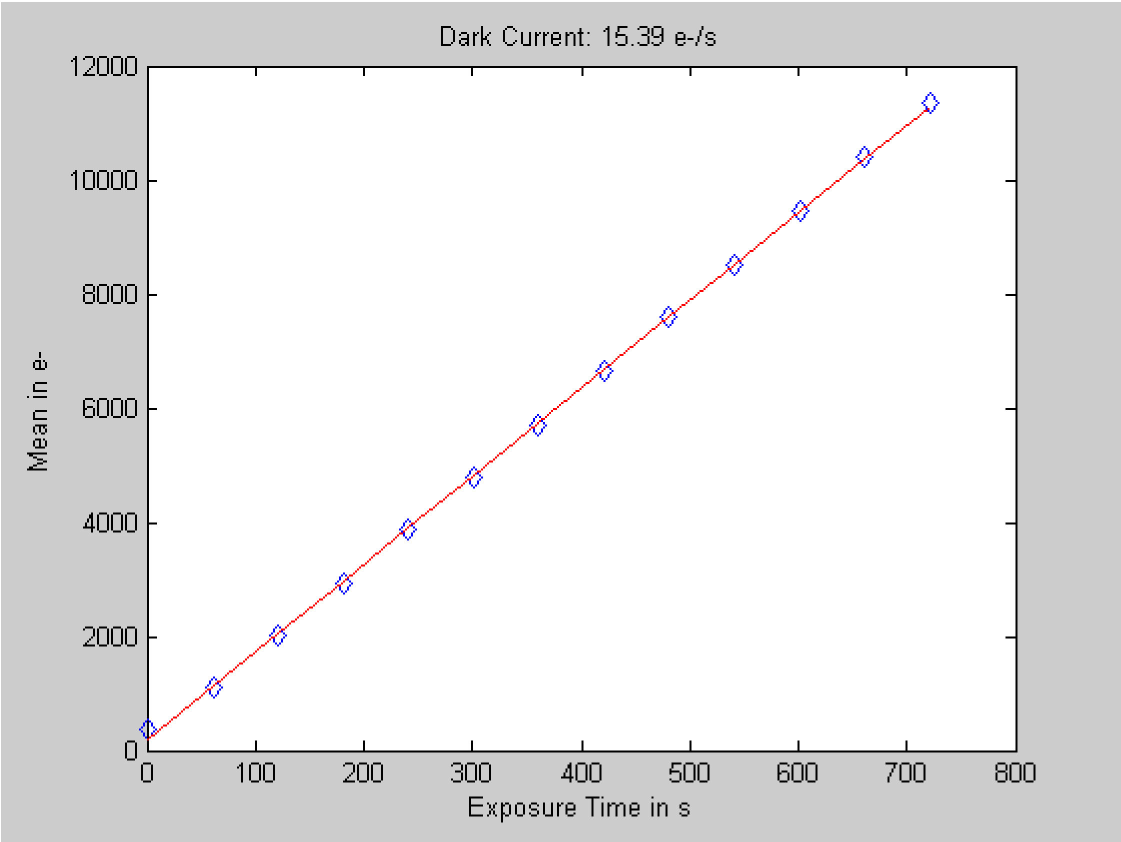


Fig 10. Dark current plot.

Linear regression is used to find the dark current to be about 15e-/pixel-s. As the detector is in 1K mode, the pixels are binned 2x2. Therefore, for one pixel in 2K mode, the dark current one quarter the 1K mode, of about 4 e-/pixel-s. This seems a bit large, considering the CCD is cooled to -50C. Improper CCD bias voltage adjustment can account for this large dark current. Also, it is possible the CCD is not as cold as the detector electronics report.

Note that dark and noise measurements are made with non-spatially corrected data. Using spatial correction would make the read noise appear smaller, due to the low-pass filtering nature of spatial correction. This would be a good trick for selling cameras. To have more complete data, such as full well capacity, and the point spread function, an X-Ray machine is needed.

Pixel Size

It is desired to know the pixel size taking account of the optics and geometric correction. A simple way to calculate the pixel size is to use pinhole mask images and measure the number of pixels for so many rows of holes. If the pitch of the mask is known, then the pixel size can be determined. A pinhole mask image supplied by Bruker is shown in Fig. 11. This image (filename *8000_1K._br)* was taken from the Bruker detector computer.

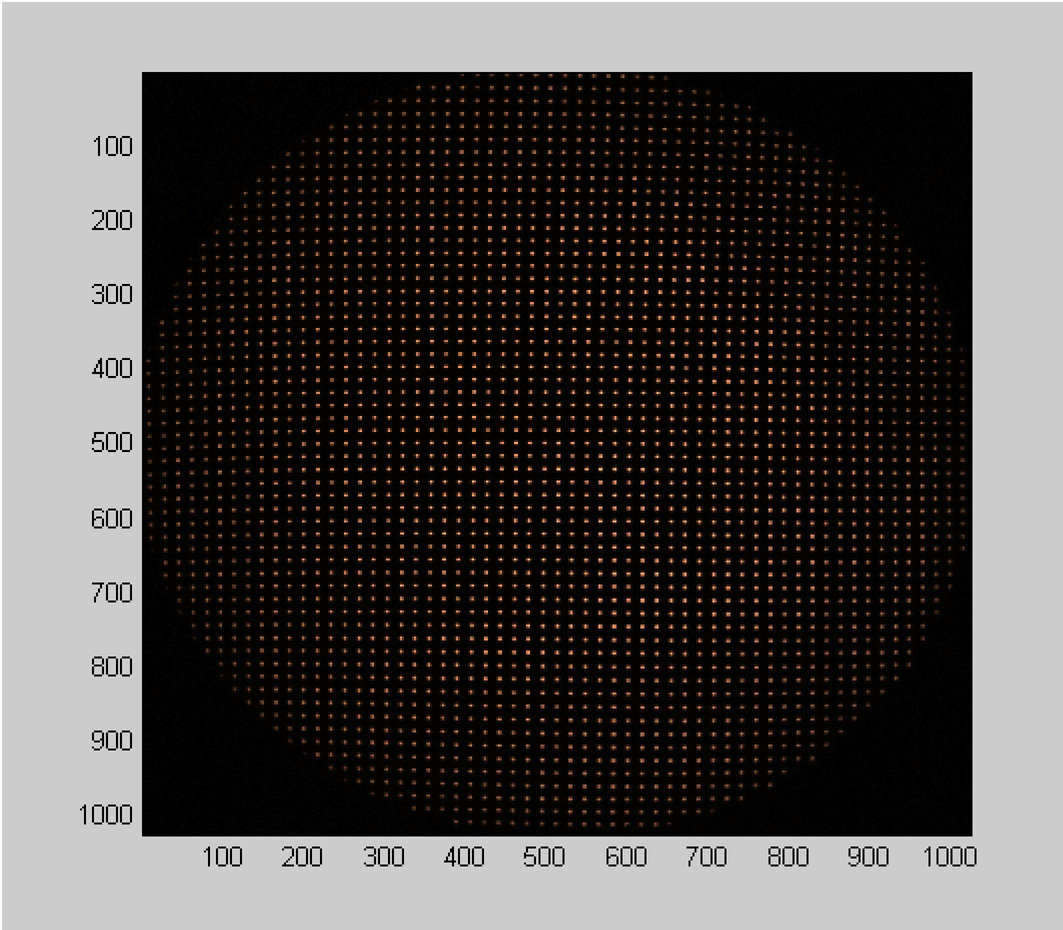


Fig. 11 Pinhole mask image from Bruker.

We can find the pixel size for the above non-spatially-corrected image by measuring the distance between the pinholes. This was done by writing a recursive algorithm to locate all of the holes, organizing the holes into rows and columns, and measuring the average distance between the holes. A pinhole image with all of the holes located is shown in Fig. 12. Note the horizontal and vertical lines added to denote that the computer found the hole, and determined its proper row and column.

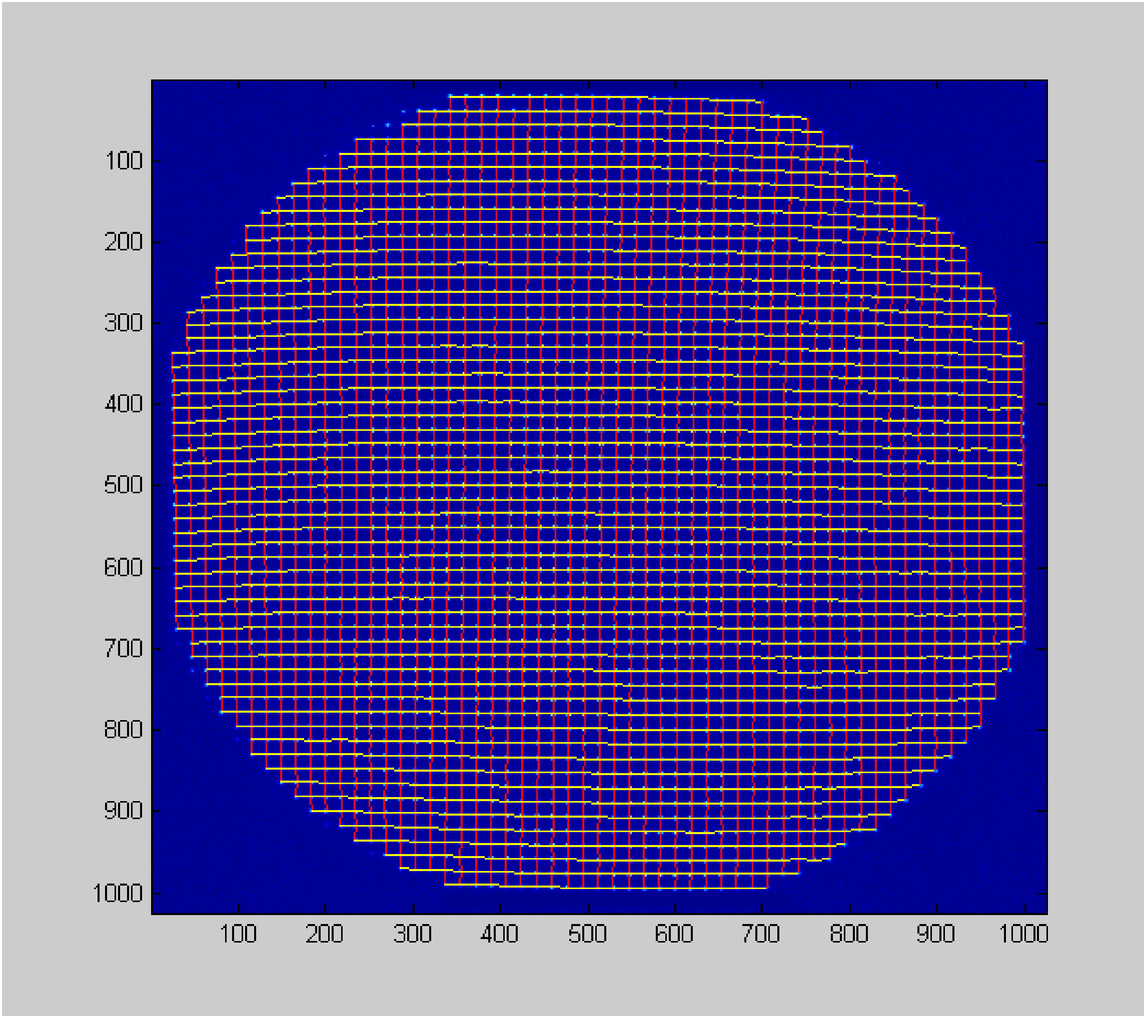


Fig 12. Pinhole image with holes located and organized into rows and columns.

Once we have a software structure of all the holes, we can calculate the linear pixel size along rows and columns. This can be plotted to show the pixel size across the face of the detector. This is a measure of the amount of geometric distortion in the image. Also, the average pixel size can be determined. The horizontal and vertical pixel sizes are plotted in Figs 13. and 14.

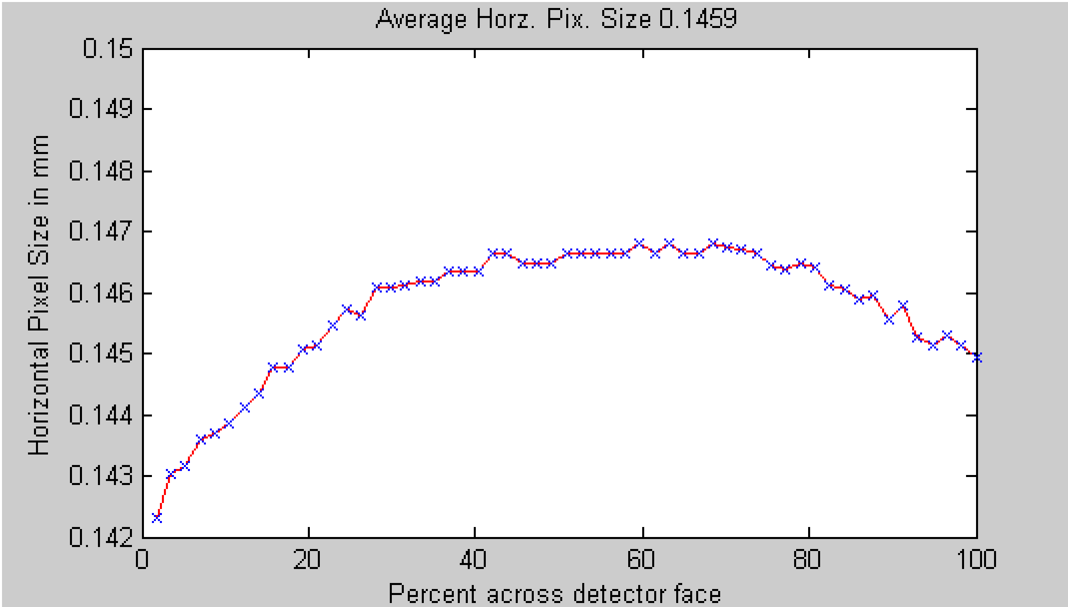


Fig 13. Horizontal Pixel size across the face of the detector. Note the pixel size is largest in detector center.

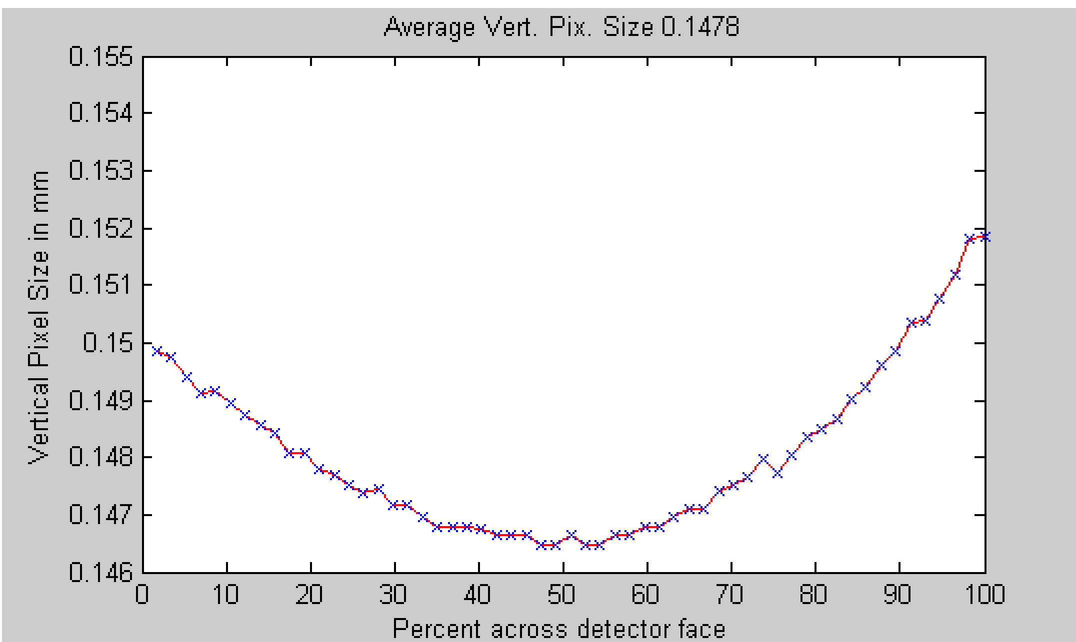


Fig 14. Vertical pixel size across face of detector. Note that pixel size is larges at edges of detector. Distortion is opposite of in Fig. 13.

Remarkably, the geometric distortion operates differently horizontally and vertically, as can be seen for Fig. 13 and 14. *As this is odd, it should be verified that these results are correct.* However, close inspection of Fig 12 seems to back up this result. The average pixel sizes are given in the plots (Fig. 13,14) at the top, for 0.146mm and 0.148mm. We can safely say the pixel size is 0.147mm.

The pinhole image was spatially corrected to tell how the spatial correction changes the pixel size. Also in plotting the pixel size across the face of the detector, we then have a measure of the accuracy of the correction. The corrected image is shown in Fig. 15.

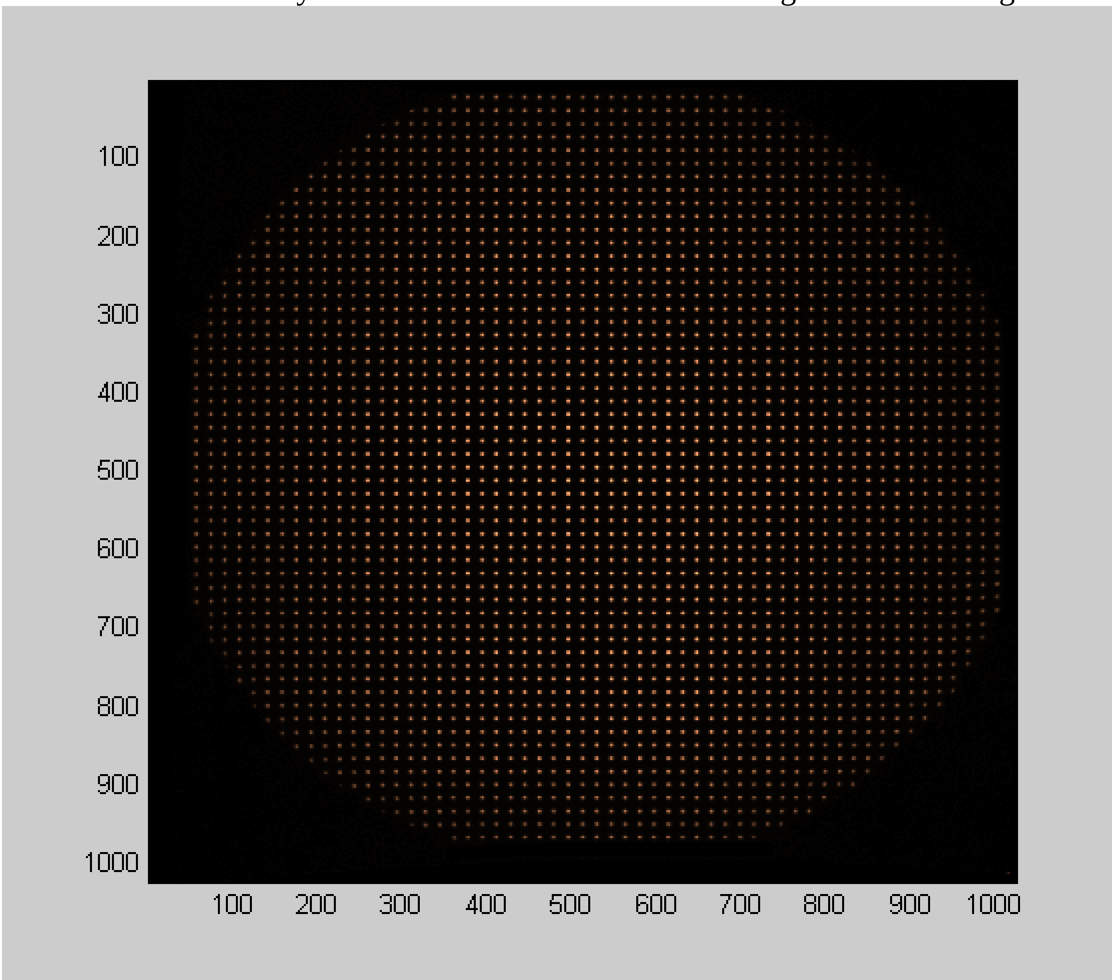


Fig. 15. Spatially corrected pinhole image.

The same image with all the holes located is in Fig. 16.

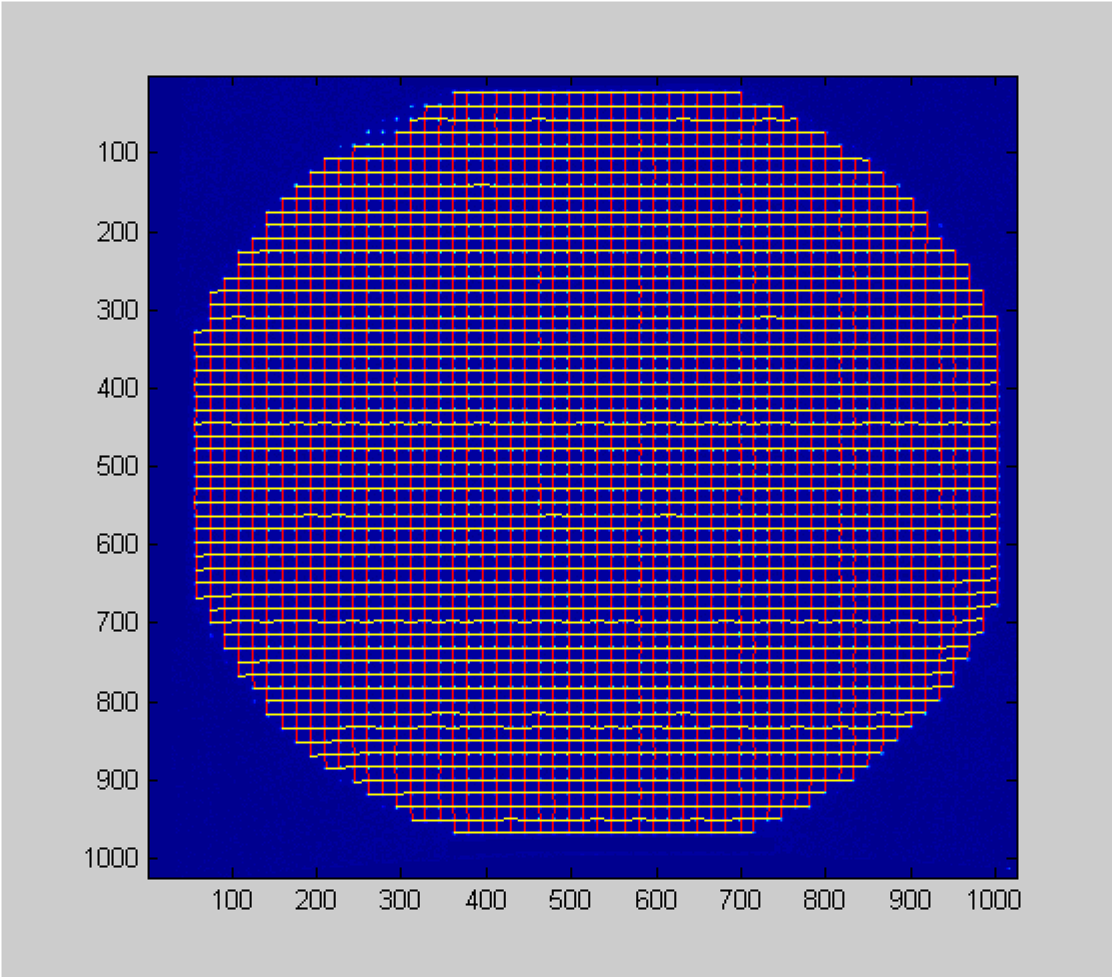


Fig. 16. Spatially corrected pinhole image with holes located.

Plotting horizontal and vertical pixel size gives Figs. 17 and 18.

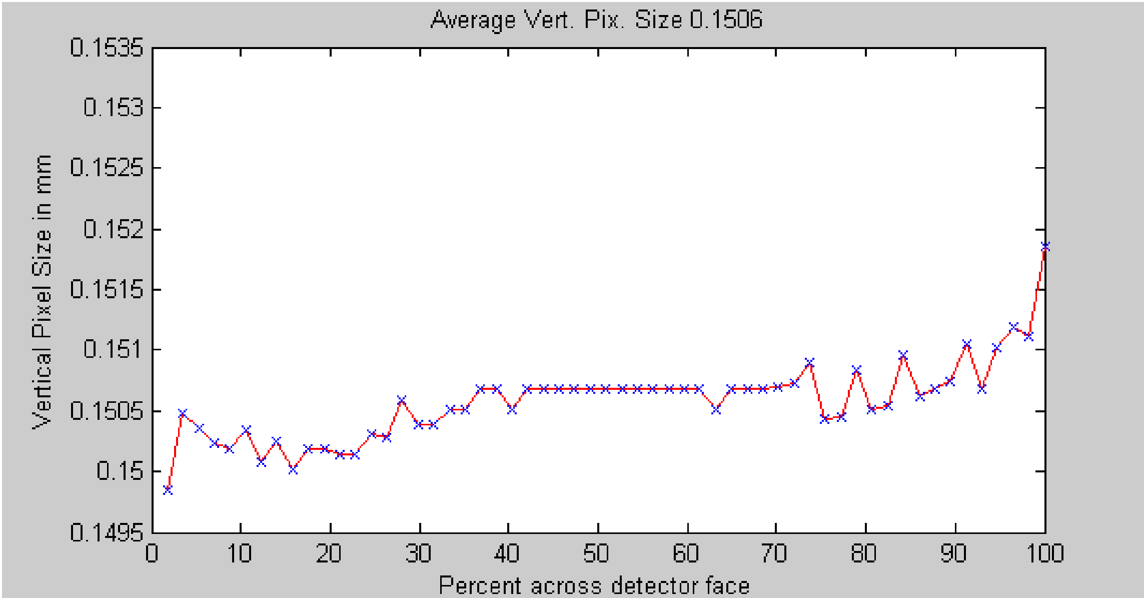


Fig. 17. Vertical pixel size across face of detector.

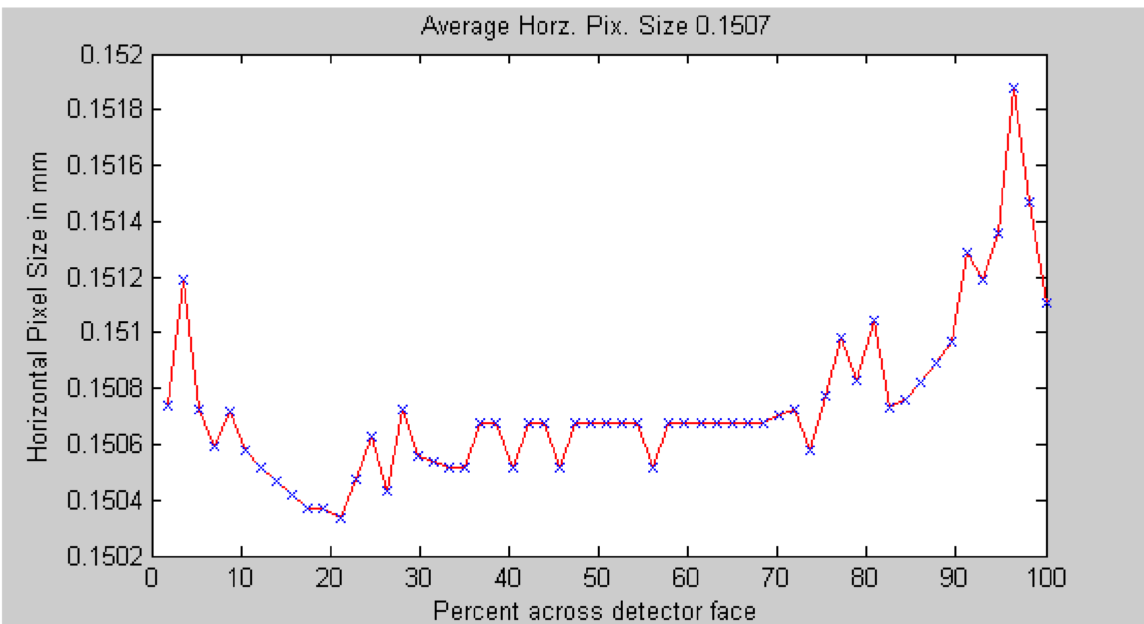


Fig. 18. Horizontal pixel size across face of detector.

After correction, we have a pixel size of .151mm.

To find the pixel size in 2K mode, we perform the same calculation to plot pixel sizes in Fig. 19. From the plots, the pixel size in 2K mode uncorrected is about 0.073mm.

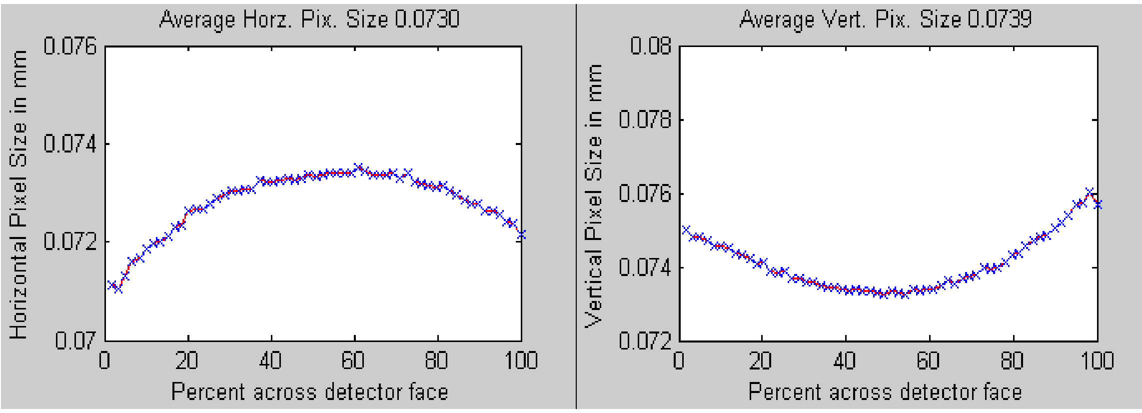


Fig. 19. Uncorrected pixel size for 2K mode.

When the image is corrected we have the image of Fig. 20.

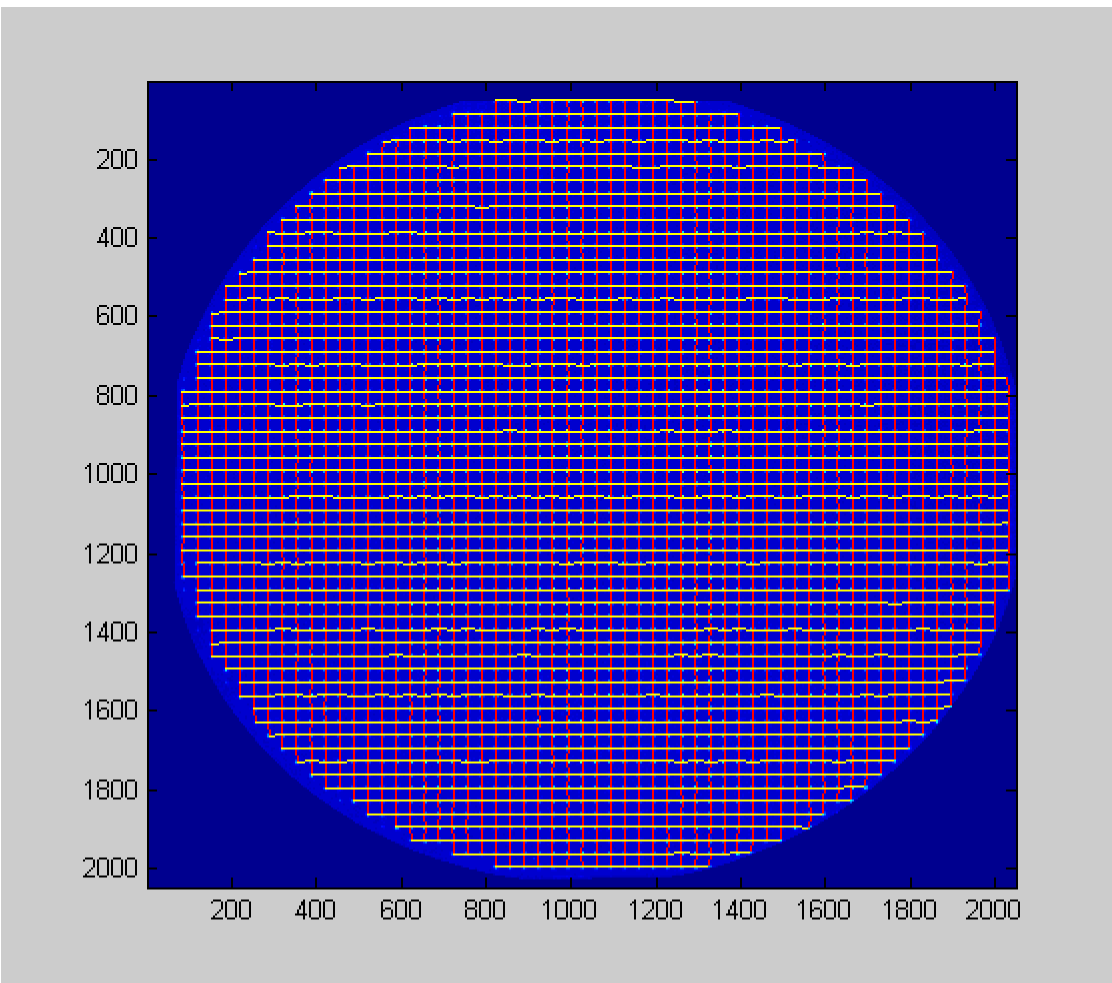


Fig 20. Corrected 2K image with holes located.

The plots of pixel size are in Fig 21. The corrected pixel size is 0.076mm.

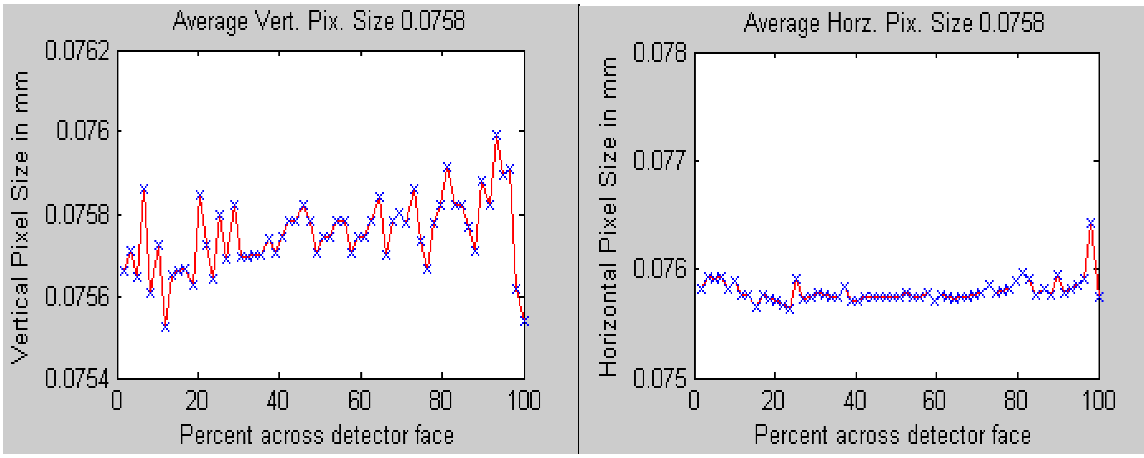


Fig. 21. Pixel size for 2K corrected image.

Distance between X-Ray source and detector-*"Distance Factor"*

When Bruker took their pinhole images, used in this pixel size calculation, they specify the distance between the X-Ray source and the detector in calibration files (specifically the *.ix file). The pinhole mask is mounted 16mm from the face of the camera due to its mechanical construction. According to the 1K mode calibration file (*.ix) the source was 20cm from the face of the camera. This means that the pinhole image will spread when projected on the phosphor by (20cm+1.6cm)/200cm=1.08. This means that the pixel size calculated above must be multiplied by 1.08. For the 2K mode, the distance is 22cm, so the scale factor is (22cm+1.6cm)/22 = 1.07. Therefore, including this adjustment, the 1K corrected pixel size is 0.163mm, and the 2K size is 0.081. Let us refer to this scale factor as the *"distance factor."*

Uncertainty in Bruker's Geometric Correction.

A major problem with Bruker's spatial correction appears occasionally, in which the corrected image is magnified. An example is taking the correction of Fig. 5 to generate Fig. 7. Another correction of Fig 5 was taken, and a magnified image in Fig. 22. appears. Clearly, the pixel size is greatly effected by this correction. Unfortunately, there is some misunderstood mode of operation in the Smart software causing the correction to magnify the image.

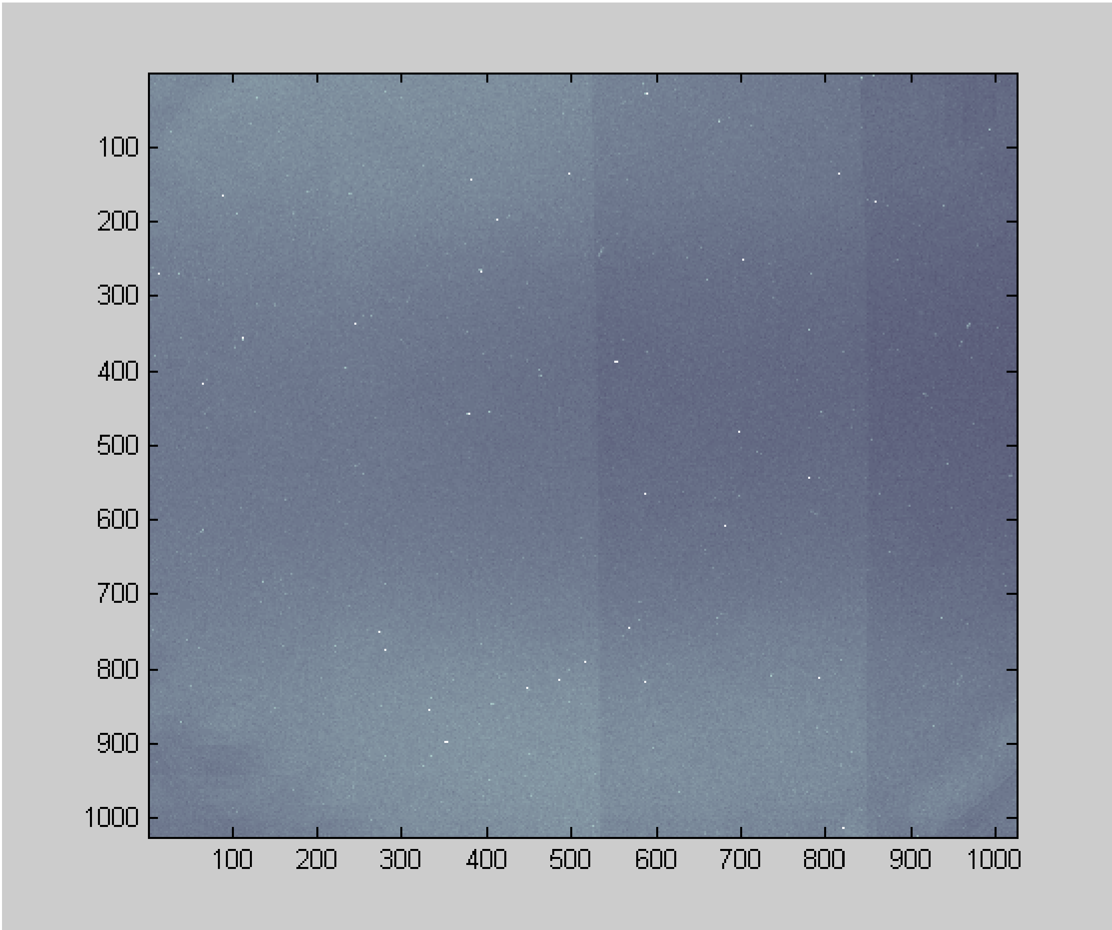


Fig. 22 Another geometric correction of Fig. 5. Comparing to Fig 7 reveals that the correction has several different unknown settings which effect the pixel size.

If this correction is applied to a pinhole image in 1K mode we get the image of Fig. 23.

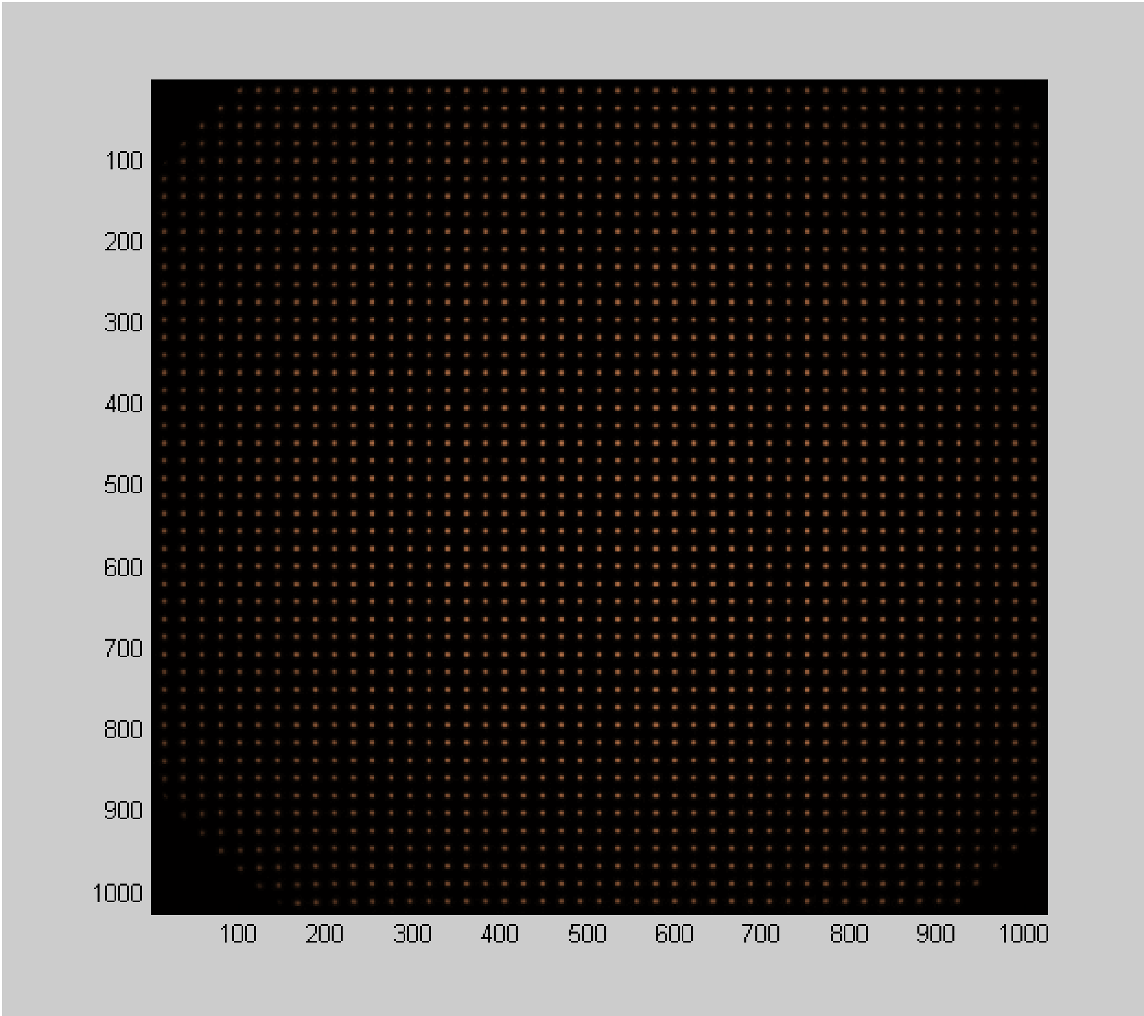


Fig 23. Enlarged and corrected pinhole image.

To calculate the pixel size in the enlarged image, we find the holes and calculate the average distances. The image with the located holes is in Fig. 24.

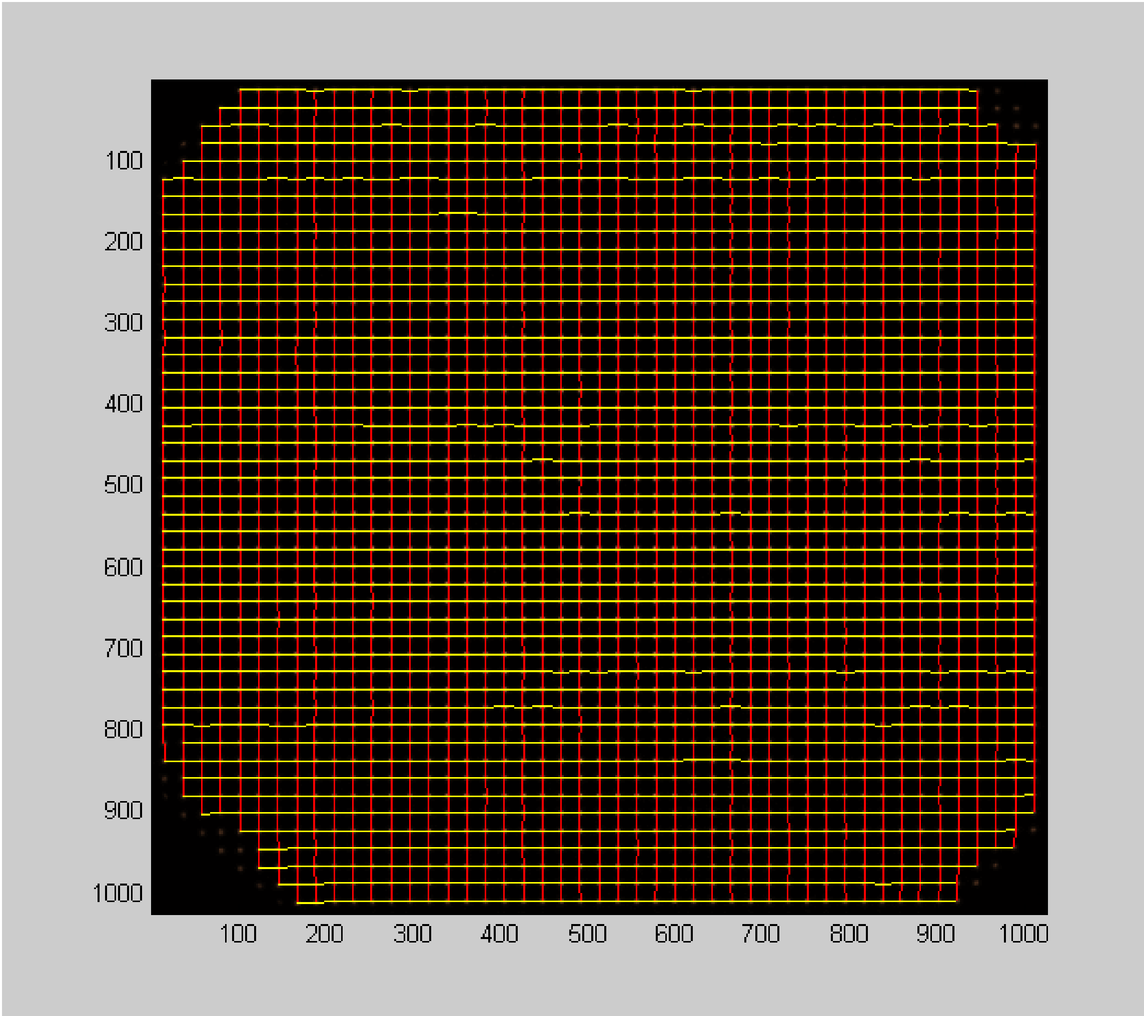


Fig 24. Pinhole mask after geometric correction. Compare this image with Fig. 16.

The pixel sizes are plotted in Fig 25 to show the pixel size to be 0.117.

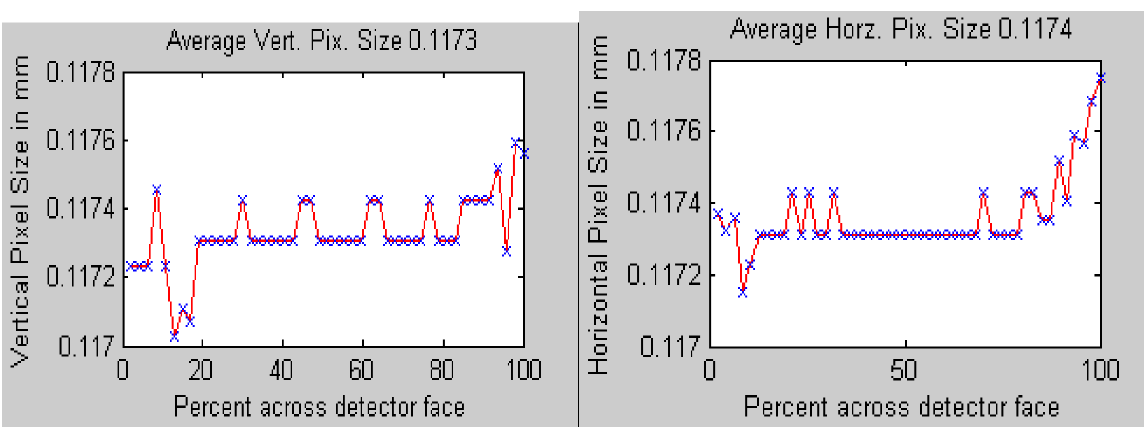


Fig 25. Pixel size plotted across face of detector, using correction in Fig. 24.

In summary, the pinhole image of Fig. 11 was spatially corrected to yield two different results for the pixel size: .117 and .151. This varies by a large 22%. This is caused by some unknown software setting. As the pixel size is crucial for any science using the detector, we must have Bruker resolve this issue.

Bruker's Specs

Bruker tested the camera system when they shipped it to ANL in 2001. The specs they claimed in shipping are as follows:

Dark Current: .46e/pixel-s (Non-MPP)
Read Noise: 47e-

We have measured much larger dark currents and read noise. This may be because the camera is out of calibration, or has aged and needs repairs. Unfortunately Bruker did not supply a spec for pixel size. This is a problem because it is extremely important for knowing the distance between Bragg peaks.

Conclusion

Dark current, read noise, gain and pixel size were measured on the Bruker detector using dark images and stored calibration files (the pinhole image). As no X-Rays were available for these measurements, we do not have measurements of full-well capacity, or more accurate measurements of pixel size. As only the 1K mode was tested, it would be useful to take data in the 2K mode. It would be beneficial to take flood field images and pinhole mask images with X-Rays to get more accurate data. In general the measured performance is worse than the specs supplied by Bruker. This may be due to the fact that the Bruker specs were supplied when the camera was new.

Appendix

Given random process X, the accumulation of dark charge on a CCD, the mean is

μ=E[X].

The variance of X is

$\sigma^2=E[X^2]-\{E[X]\}^2$.

With electronics gain of A, the mean of the electronics output is

$E[AX]=AE[X] = A\mu$.

The variance at the output is now

$E[(AX)^2]-\{E[AX]\}^2=A^2E[X^2]-A^2\{E[X]\}^2=A^2\{E[X^2]-\{E[X]\}^2\}=A^2\sigma^2$.

See [Stark and Woods, *Probability, Random Processes, and Estimation Theory for Engineers,* Prentice Hall, 1994, pp. 162-163.] for reference.