Case Study: Custom CCD for X-ray Free Electron Laser Experiment

Introduction

The first XFEL (X-ray Free Electron Laser) experiments are being constructed around the world. These facilities produce femto-second long bursts of the most intense coherent X-rays ever to have been produced, with the individual pulses repeating at a frequency of 5-120 Hz depending on the experiment.

The beam intensities are such that samples which are illuminated can be instantly destroyed, but in the fraction of a second (down to sub ps) before this occurs, a diffraction pattern may be recorded providing insight and knowledge into the molecular structure of the samples that are tested. Uniquely, it is possible to obtain diffraction patterns of non-crystalline substances, before the sample is destroyed, essentially providing atomic level movies of the sample under investigation. The diffraction patterns created can be very intense in the centre close to the beam, but contain faint detail in the outer parts of the pattern that are critical for the complete understanding of the sample structure; furthermore the diffraction patterns require a relatively large area detector. Realising a detector that is suitable for such experiments presents a challenge, but is one that can be met with a new CCD design.

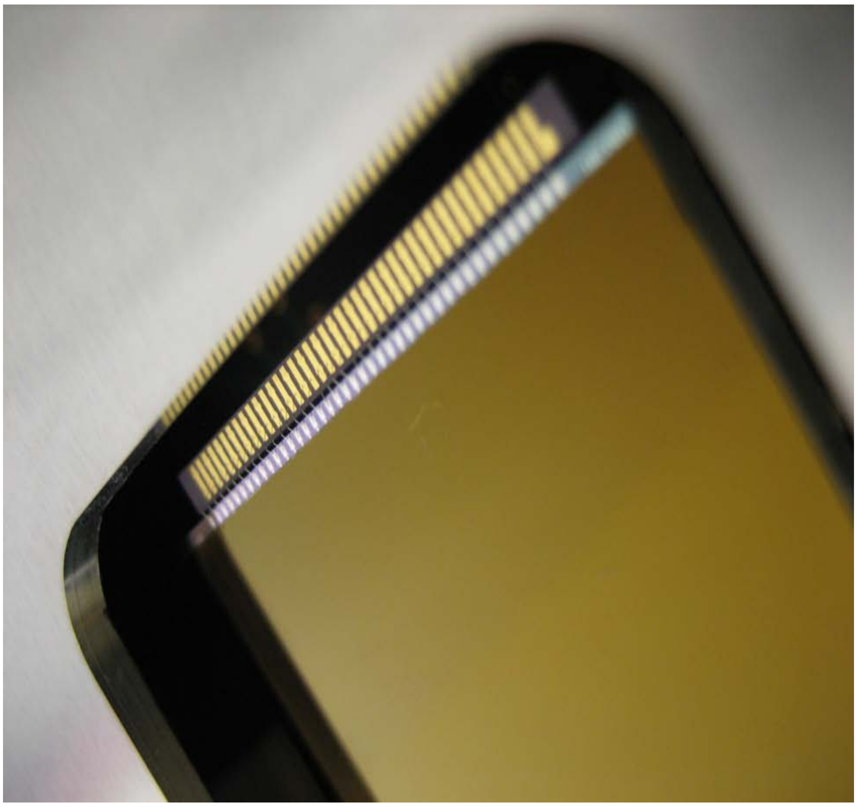

Fig 1: Very Large Area e2v technologies CCD

Dr. Takaki Hatsui, scientist at the Japanese XFEL facility at Spring8, Japan, contacted XCAM for some advice and assistance, when he realised that a CCD detector might provide a solution to his sensor requirements, if only he could create a custom CCD which encompassed the relevant characteristics that he required.

He knew that different CCD types each individually had desirable characteristics, but no CCD offered all of the specific characteristics encompassed in one detector. In particular the ability to handle the large signals close to the beam from the intense X-ray pulse was a concern. He wondered if XCAM would be willing to investigate the options available and perform some tests to evaluate some of the unknown performance issues, culminating in a custom sensor specification that could be presented to sensor manufacturers as a basis for procurement.

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Review of CCD Options for XFEL

XCAM started the work by reviewing both the requirements for an XFEL detector and examining the CCD characteristics which would best meet these requirements

Finding a detector suitable for capturing the diffraction patterns that are produced by these experiments was challenging. A suitable detector ideally needed the following characteristics:

- The primary, and most challenging requirement, would be the ability for each pixel to hold the signal from up to 1000 12 keV X-rays per pixel. This would require a pixel well capacity of at least 3M electrons (most scientific CCDs have full well capacities <500k electrons)
- A suitable detector would need large area in order to capture the full extent of the diffraction pattern
- Read-out speeds of the large area CCDs would be required at frame rates consistent with the 60Hz repetition rate of the beam for best use of this expensive facility (most large area CCDs only operate at ~1 Hz)
- The CCD would need to be able to withstand the X-ray radiation for a suitably long period of time before it would require replacement, with a goal of typically 1 year operation before replacement is needed
- The ideal detector would need to have the capability to detect single X-ray photons in the outer parts of the diffraction pattern, whilst detecting beams of high intensity in the centre of the pattern impacting on the total system noise
- The energy of the beam would be 6-12 keV
- The resulting camera head would need to be suitable for clean ‘in-vacuum’ operation

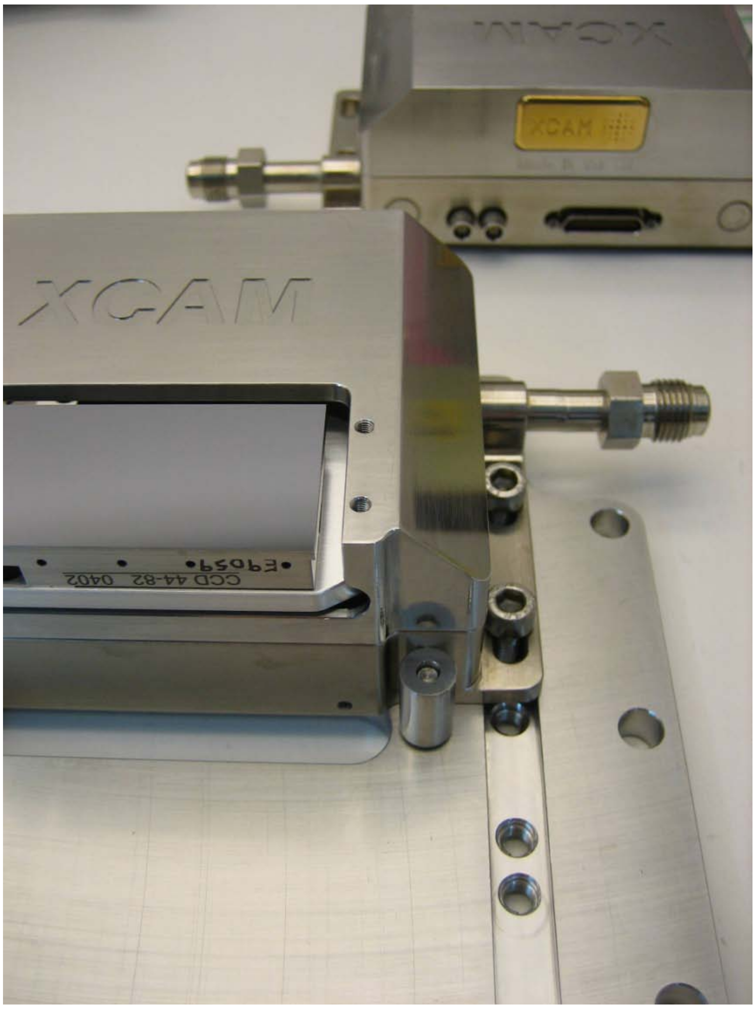

Fig 2: Large Area CCD Camera Constructed for an XFEL Experiment already in operation

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XCAM came up with a CCD concept which encompassed all of the above in a single detector, and specified an initial value for each technical specification and addressed the key issues which would need further investigation.

Areas which were thought to require further careful examination and study were as follows

- **Radiation Damage**: CCDs were not designed to operate with such high X-ray doses which amounted to in excess of 50 Mrad/yr close to the beam axis; one of the important aspects of the study which needed testing at an early stage, therefore, were the radiation damage mechanisms which might occur when the CCD was subjected to the levels of X-ray dose that they might see when used for an XFEL experiment.
- **Spatial Resolution under the Intense X-ray Pulse**: One of the key concerns with silicon imaging technology was related to the generation of a sudden huge signal in the pixels, which was significantly greater than the device doping concentrations, and which would subsequently destroy the electric fields within the device, creating a very poor spatial resolution, in which the intense diffraction peaks were essentially "blurred".
- **High Full Well Capacity**: CCDs traditionally have been used in very low signal applications and part of the custom design would involve ensuring that the pixels of the custom sensor would have a high full well capacity.
- **High Frame Rates with Low Enough Noise**: The 60Hz repetition rate of the XFEL pulse required a custom large area CCD that operated at 60Hz, but a good noise performance would still be required.

Radiation Damage Study

In order to test radiation damage, a very simple, low cost camera head was constructed using representative standard e2v Technologies CCD30-11s. The devices were thoroughly characterised at XCAM and an irradiation plan was agreed with the customer who then arranged for the device to be irradiated in such a way that the device received incremental doses which were representative of the dose that the device might be expected to experience during a year's use in the experiment.

The device was then returned to XCAM who re-characterised the device before issuing a report on the effects of the X-ray radiation damage. Recommendations were made impacting the electronic system design, to enable the early effects of radiation damage to be ameliorated by changes in operating conditions, so extending the useful life of the devices.

The results of this work were taken into consideration when specifying the custom sensor, and the work will be published in due course. The results demonstrate that the CCD technology can be used in the XFEL application taking scientific data for up to a year of normal operation.

Annual Dose Equivalents

0.1 0.3 0.1 0.3 1.0

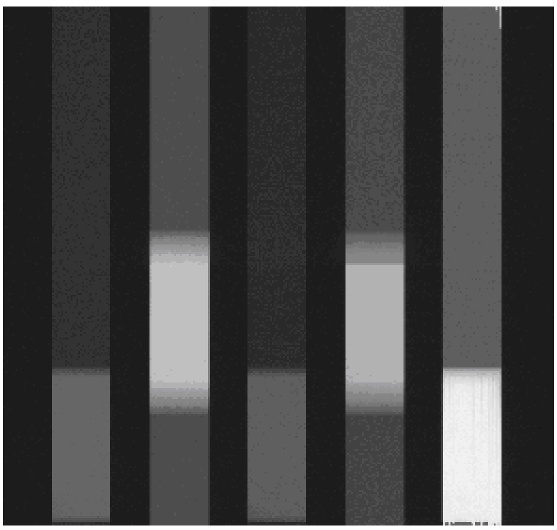

Fig 3: Leakage Pattern in Irradiated CCD47 used for Radiation Damage Study

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High Signal Handling Capacity

In order to study issues such as high full well capacity and high signal handling capacity on the output node, a standard CCD38 (Dental CCD) which had been designed for high signal-handling abilities was tested. Predictions were made for differing pixel and amplifier configurations such that in the final design, a signal handling capability of >5 M electrons per CCD pixel was designed. In use, these pixels could be digitally binned 2x2 producing image pixels each containing in excess of 20 M electrons per 100 μm pixel, and capable of sampling up to 6000 X-rays of 12keV. This was significantly in excess of the initial goal of sampling at least 1000 X-rays and was one of the significant developments which enabled the custom camera project to proceed.

Linearity and PSF testing

There were initially concerns that the signal generated by the intense X-ray pulse would collapse the potential wells which defined the pixels, leading to degraded spatial resolution. XCAM set about evaluating the behaviour of the CCDs under the intense X-ray pulse which lasts approximately 5 fs. XCAM also performed testing at the Spring-8 synchrotron to explore the charge storage behaviour for very large signals. As a result of the work it was possible to demonstrate that for the MOS CCDs manufactured by e2v technologies, there would be no appreciable degradation in the point spread function (PSF) arising from the intense signal generated in a few ns. Again, this finding helped reduce the technical risk of developing a custom CCD imaging solution for the XFEL.

Evaluation of Radiation Hard Devices to Test their Suitability

E2v Technologies produce some CCDs manufactured using proprietary processes to make them more tolerant to radiation damage. However, radiation damage is usually assessed using gamma rays (e.g. from Co-60) where the characteristics of the radiation are significantly different to that expected in an XFEL experiment (6-12 keV photons). For this reason, samples of standard process and radiation hard CCDs were obtained and evaluated to establish if these processes should be considered for the custom CCD. The devices were tested in pseudo-logarithmic increments up to an anticipated annual dose equivalent to 50 Mrads, and were found to operate satisfactorily afterwards, albeit requiring some modest cooling to reduce the excess noise introduced by an increase in leakage current. This work demonstrated that the CCD devices could be used satisfactorily for periods up to a year in routine operation, and also fed into a spares policy to be used on the synchrotron.

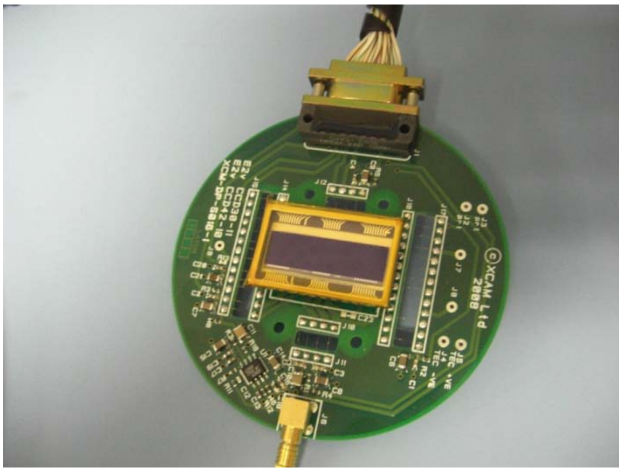

Fig 4: (Left) The CCD38 used for evaluation of high signal handling capacity CCDs, and (right) the CCD30-11 used for radiation damage studies

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Custom Sensor Specification

The various work packages, once completed, enabled XCAM to produce a specification for a custom sensor, for which a contract was awarded to e2v technologies in March 2009 (see http://www.e2v.com/news/e2v-components-power-japan-s-biggest-scientific-project/) for the press release with further details.

I am a team leader of the Data Acquisition team for the Japanese X-ray Free-Electron Laser (XFEL) project. http://www.riken.jp/XFEL/eng/index.html

My role is to construct the data acquisition infrastructure by 2011, which is the year that the first user time of our XFEL will be scheduled, giving birth to x-ray free-electron laser science. One of the key components of the experimental system is the 2 dimensional x-ray detector for XFEL. Without the detector, we will be in a situation where the laser beam illuminates a completely novel scientific field without us having the eyes to observe it.
As the characteristics of XFEL light is so different from the light available from current x-ray generation technologies, we needed to establish the detector concept from scratch.

Before coming to Riken I was an assistant professor at Institute for Molecular Science, Japan, and XCAM worked with me at that time to build a unique camera based on an L3 CCD for my soft x-ray experiment, achieving an unprecedented resolution of 3 microns. Having worked with XCAM previously, I realised that they had the expertise that I needed in order to investigate options for the XFEL detector. The collaboration with XCAM Ltd on the XFEL work started in 2007. At that time I had some simple equations telling me that custom CCD devices with a combination of state-of-the-art technologies would be a great option for our project. I was excited at the new idea, but I was also aware that there were many critical concerns, such as the device reliability under extremely brilliant pulsed x-ray irradiation, and the probability of performance degradation due to the as yet unknown physics involved in detecting ultra-short intense pulsed x-rays, which no human being had created before.

To address these concerns, XCAM Ltd worked with us to produce a complete survey of the current CCD technologies, and they completed feasibility studies, which included the production of a custom camera for the experiments, evaluation of radiation damage, which is critical in estimating the life of the devices, and recommendation of the custom device specifications.

Owing to the outstanding and unrivalled ability of XCAM Ltd, we successfully launched the development project of a novel CCD detector dedicated to our XFEL on March 18th, 2009. We all thank XCAM Ltd for their crucial and enthusiastic contributions.

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