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Femtosecond Radiation Experiment Detector for X-ray Free-Electron Laser (XFEL) Coherent X-ray Imaging

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Abstract-A pixel array detector (PAD) is being developed at Cornell University for the collection of diffuse diffraction data in anticipation of coherent x-ray imaging experiments that will be conducted at the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center (SLAC). The detector is designed to collect x-rays scattered from femtosecond pulses produced by the LCLS x-ray laser at framing rates up to 120 Hz. Because x-rays will arrive on femtosecond time scales, the detector must be able to deal with instantaneous count-rates in excess of 10¹⁷ photons per second per pixel. A low-noise integrating front-end allows the detector to simultaneously distinguish single photon events in low-flux regions of the diffraction pattern while recording up to several thousand x-rays per pixel in more intense regions. The detector features a per-pixel programmable twolevel gain control that can be used to create an arbitrary 2-D, two-level gain pattern across the detector; massively parallel 14bit in-pixel digitization; and frame rates in excess of 120 Hz. The first full-scale detector will be 758 x 758 pixels with a pixel size of 110 x 110 microns made by tiling CMOS ASICs that are bumpbonded to high-resistivity silicon diodes. X-ray testing data of the first 185 x 194 pixel bump-bonded ASICs is presented. The measurements presented include confirmation of single photon sensitivity, pixel response profiles indicating a nearly single-pixel point spread function, radiation damage measurements and noise performance.

I. INTRODUCTION

N EW high-intensity x-ray sources like X-ray Free-Electron Lasers (XFEL) are opening new possibilities into the types of x-ray studies that can be performed. It is anticipated that intense, femtosecond time-scale pulses produced by XFELs will make the direct study of single particle electron density structure possible [1]. Even though the energy absorbed by a particle during an ultra-intense XFEL pulse will destroy its chemical structure because of massive ionization and a subsequent Coulomb explosion of the sample, a pulse that is short enough should still yield relevant scattering information directly related to the original electron density of the particle. This is because the Coulomb explosion of the particle is rate limited by the acceleration of ionized

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S. M. Gruner is with Cornell University, Laboratory of Atomic and Solid State Physics, Ithaca, NY 14850 USA, and is director of Cornell's High Energy Synchrotron Source (CHESS) (telephone: 607-255-3441, email: smg26@cornell.edu). particles/atoms. If the pulse is short enough, the x-rays are scattered before the Coulomb explosion occurs.

The experimental set-up, collection of data, and analysis of the collected data are non-trivial. Even if the x-ray pulse is short enough in duration and intense enough to produce the desired scattering pattern, other technological issues are noteworthy and critical to the success of the experiment, including arranging temporal and spatial overlap of very short pulses and single particles, the orientation of the particles in the x-ray beam, and the best x-ray data collection strategy. Complicating matters, many frames of valid scattering data are needed to reconstruct the original particle because much of the scattering pattern, particularly in important high-q (large scattering angle) regions, will be extremely low flux. For the experiment being considered, the expected flux in these regions is less than one photon per pixel. Another difficulty is that in most single particle scattering schemes, the orientation of the particle is not determined and the scattering patterns must be classified after the fact based on similarities of the scattering patterns themselves.

The pixel array detector presented here is one answer to the technological question of how to collect the scattering patterns for the coherent x-ray imaging (CXI) of single particles at the Linac Coherent Light Source (LCLS) XFEL. Many of the detector characteristics are tailored specifically for the demands of the experiment, some of which are mentioned above. Specific technical requirements include the ability to distinguish whether or not single x-ray photons have been detected in any given pixel while maintaining the ability to detect thousands (>2500) of x-rays per pixel in other parts of the scattering pattern. This is particularly notable since for a pulse that approaches 10 fs in length, the instantaneous count rate for some pixels will be greater than 10^{17} photons per second. This count rate alone excludes the possibility of using a photon counting detector. Another notable technical requirement, related to the ability to distinguish single photons, is a pixel-limited point spread function. In addition, the detector must be able to sustain a continuous frame-rate of 120 Hz. This follows from the operating procedures planned for the LCLS, and the high number of frames required for reconstructing the electron density from the diffuse x-ray scattering patterns produced by coherent x-ray imaging of noncrystalline samples.



Fig. 1. High-level schematic of the pixel showing the major functional components: The front-end amplifier, the sample-and-hold buffer, and the digitization components. In addition to these basic functional units, the in-pixel programmable gain mechanism is shown. The digitization method is similar to that presented in reference [3].

II. PHYSICAL CONSTRUCTION OF PIXEL ARRAY DETECTOR (PAD)

A PAD is composed of two layers, the detector layer and the signal processing layer. These layers are mated together with isolated, pixel-level connections using solder bump-bonding¹. The detector layer is an array of diodes² made from 500 μ m thick high-resistivity $(5-10 \text{ k}\Omega)$ n-type silicon. The thickness of the diode layer gives a high quantum efficiency, greater than 0.99, when detecting 8 keV x-rays. The high resistivity of the diodes ensure over-depletion when a bias voltage of 200 volts is applied. In operation, incident x-rays are absorbed by the silicon in the diodes and converted into charge carrier pairs. These charges migrate according to the applied electric field and the respective mobilities of the charge carriers. For the PAD presented, holes are collected (reasons for this are explained elsewhere [2]) by the signal processing layer through pixel-level connections. The signal processing layer is a 0.25 micron CMOS, mixed-mode application specific integrated circuit (ASIC) manufactured by TSMC³. Each pixel of the ASIC has dedicated circuitry for processing the charge collected from the diode. The pitch of the pixel connections across the 2-D detector array is $110 \,\mu\text{m}$. The size of the single pixel layout in the CMOS ASIC corresponds to the pitch (i.e. the pixel size is $110 \,\mu m \times 110 \,\mu m$).

III. PIXEL-LEVEL DESIGN AND OPERATION

A. Pixel Operation Description

A high-level schematic of the pixel is shown in figure 1. X-ray induced charge in the diode is collected at the 'in' node and integrated onto the feedback capacitance of the frontend capacitive transimpedance amplifier. The total feedback capacitance can be set to either the capacitance of cap1 or the sum of cap1 and cap2 to configure the gain (volts per integrated unit of charge) of the front-end. The selection of the capacitance is determined by 1-bit in-pixel memory that can be individually programmed for each pixel in the array.



Fig. 2. A simplified timing diagram of the detector showing a division between exposure time, digitization, and detector readout. The planned exposure time for the CXI experiment is $10 \, \mu s$. The digitization time is approximately 4 ms and the readout of the ASIC takes 3.2 ms. A frame rate of $120 \, \text{Hz}$ (period 8.3 ms) is easily achieved with this timing division.

The capacitance of the feedback loop with and without cap2 as part of the integrating feedback loop is $565 \, \text{fF}$ and $75 \, \text{fF}$, respectively. Since x-ray conversion in silicon produces 1 electron per 3.65 eV of absorbed energy, the gain of the front-end stage is either 0.62 mV per 8-keV x-ray (low gain) or 4.7 mV per 8-keV x-ray (high gain). Since the usable voltage range of a pixel's analog stage is conservatively set to 1.7 V (set by the ramp, the digitization clock and Vref), the saturation of the pixel during normal operation is approximately 2700 x-rays in low-gain and 360 x-rays in high-gain.

After the charge is integrated by the front-end, the voltage at node A is sampled by the sample-and-hold stage and held constant during the next stage of in-pixel data acquisition, which is digitization.

During digitization, the voltage at node B is compared to a globally transmitted ramp while a global analog-to-digital conversion (ADC) clock increments an in-pixel 14-bit counter. When the voltage of the ramp crosses the the voltage held at node B, the counter is disabled and the value of the counter is taken to be proportional to the total charge integrated by the pixel. The digitized value of each pixel is then shifted onto a digital bus with a readout clock. These values are the output of the PAD.

B. Waveforms and Pixel Timing

Figure 2 shows a simplified timing diagram for the pixel operating in a mode compatible with the requirements of the LCLS CXI experiment. The integration time shown is a small fraction of the framing period and in normal operation only spans $10 \,\mu$ s. After the integration time, the output voltage is sampled and digitized. Digitization in normal operation takes 4 ms, occurring simultaneously for all pixels. Pixel readout then proceeds and requires addressing (not shown in figure 2). Each pixel is addressed and readout by switching the counter to act as a shift-register.

IV. CHIP-LEVEL ARCHITECTURE

The 2-D detector array comprises 8 banks of identical pixels with every column being a mirror image of its nearest neighbor columns for efficient sharing of digital and analog buses on the ASIC. The general structure is shown in figure 3. Seven

¹Bump bonding done by RTI, International Center for Materials and Electronic Technologies, Research Triangle Park, NC, USA

²Detector diode manufactured by SINTEF, NO-7465 Trondheim, Norway ³Taiwan Semiconductor Manufacturing Company Limited, No. 25, Li-Hsin Rd., Hsinchu Science Park, Hsin-Chu, Taiwan 300



Fig. 3. Chip level architecture: The pixels are grouped in eight banks (N=8). Each bank has a dedicated digital output. Addressing is achieved by using two bit passing addressing shift-registers. The column-addressing shift-register is fanned out to all banks so that the corresponding columns in each bank are addressed in parallel.

of these banks are 26×185 pixels and one bank is 12×185 pixels. The total dimensions of the array itself, approximately 21 mm \times 21 mm, are constrained by limits of the die size offered by the commercial CMOS process used. The banks are addressed using two shift registers that pass a bit to activate the column or row desired. The column shift-register, which has 26 output positions, is fanned out to the eight banks so that corresponding columns in each bank are addressed in parallel. Each bank has a dedicated digital output. Full readout of the array is accomplished in 3.2 ms using a 25 MHz data clock. The output from the array is completely digital. The data acquisition process is controlled with an FPGA interface board based on the Xilinx XC4V100FX FPGA. This board provides an interface to a PCI-Express bus [4].

V. TESTING RESULTS

Bump-bonded modules have been tested and verified to be fully functional and appropriate for the experiment. Full-speed readout and real-time framing has been verified for sustained continuous acquisition of data. Figure 4 is a radiograph of part of a United States one dollar bill, verifying correct ordering of the data. Measurements of the single pixel saturation values for nominal operating conditions are in accordance with the anticipated values, namely $\approx 360~8~{\rm keV}~{\rm x}$ -rays for high-gain and $\approx 2700~8~{\rm keV}~{\rm x}$ -rays for low-gain. The signal-to-noise ratio for detecting a single 8-keV photon was measured to be approximately 7 for high-gain mode and approximately 2 for low-gain mode.

A. Single Photon Sensitivity

The PAD in the CXI experiment must faithfully record the number of photons incident on the detector in low flux regions. This requires a signal-to-noise ratio large enough to clearly distinguish quanta associated with single photon events. Figure 5A shows a histogram of the output of a single pixel in high-gain mode over more than 4000 frames with a



Fig. 4. An x-ray radiograph of a US one dollar bill. The x-ray source used was a copper anode x-ray tube. The features of the green ink on a one dollar bill are about the same size as the pixel pitch. The image contrast comes from the green ink of the dollar bill.

 $75 \,\mu\text{m}$ diameter pinhole masking most of the charge sharing regions on the pixel perimeter. The x-ray source used was an x-ray tube with a copper anode run at 14 kV, 0.7 mA. A 50 μ m thick nickel filter suppressed the bremsstrahlung spectrum and Cu K $_{\beta}$ radiation. The resulting beam was nearly monochromatic with an energy corresponding to the Cu K $_{\alpha}$ line (8.04 keV). The peaks correspond to 0, 1, 2, ... etc. 8 keV photons.

When an x-ray illuminated pinhole is positioned so that



Fig. 5. Histograms of pixel outputs over thousands of frames. Sub-figure A is from a pixel which is illuminated through a 75 micron pinhole. The pinhole reduces charge being shared with other pixels because x-rays convert only in the central region of the pixel. The result is a histogram with clearly distinguishable peaks corresponding to an integer number of photons detected. Sub-figures B and C show similar histograms of two adjacent pixels, but with the pinhole positioned to illuminate the border region between the pixels. Sub-figure D shows a histogram of the per-frame sum of the two pixels (B and C) for the same data set, and demonstrates complete measurement of deposited charge by recovering a histogram similar to sub-figure A. All pixels are in high-gain mode. Small gain corrections were applied when summing the pixels.

its projection straddles the border between two pixels, a significant number of the photons incident on the detector convert in charge sharing regions where the charge produced by an absorbed photon is split between pixels. Since only a fraction of the charge produced by a charge sharing event is collected by an individual pixel, histograms of single pixel outputs over many frames do not show a clear quantized response. This effect is shown in figure 5B and 5C. In this case, the total charge deposited by a given x-ray event remains constant and a histogram of the frame-by-frame sum of the two pixels (calculated after a small gain correction) recovers discernible x-ray peaks (5D). There is, however, a degradation in the quality of the histogram because the noise associated with the sum of pixels is greater (by a factor of $\sqrt{2}$) than the noise associated with a single pixel.

B. Line Spread Function

Directly collecting charge produced by x-rays absorbed in a fully-depleted silicon detector layer has several advantages over x-ray detector methods that rely on detecting secondary optical photons emitted by a phosphor. One of these advantages is a comparatively superb point spread function. This is because after the charge is produced, it is directly collected by the applied electric field. The spread of charge during the time it takes to migrate through the detector layer to the pixel connection may give rise to charge sharing between pixels. Measurement of charge sharing and pixel response as a function of position of incident photons can be accomplished by measuring the line spread function with a knife-edge that is held at a slight angle to the column (or row) so that varying degrees of pixel exposure are collected as a function of position along a knife edge illuminated with a flat field. Additional, finer resolution data can be gathered by translating the detector behind the x-ray illuminated knife edge. A measurement of this sort is shown in figure 6. Pixel output is plotted as a function of mean knife edge position with respect to the pixel center. The derivative of this, also shown, gives the line spread function. The line spread function recovered is the convolution of the charge spreading in one dimension with a one-dimensional box function having the same width as the pixel (110 μ m). The results of the measurements show discernible charge sharing up to 20 μm from the nominal pixel boundary. Beyond this charge sharing region, the line spread function is flat and dominated by pixelization. Since the pixels are $110\,\mu\mathrm{m}$ wide, the line spread and point spread functions are pixel-size limited. The width of the charge sharing region does, however, indicate that a significant percentage (up to 60%) of randomly distributed incident photons will be affected by charge sharing to some degree, as they will be within $20 \,\mu m$ of the pixel boundary.

C. Radiation Testing

Radiation damage of the bump-bonded pixel array detector was tested up to 75 MRad (Si) referenced to the face of the detector using an 8 keV x-ray source. The results indicate that leakage currents of the diode increase, but the impact on data collected for the proposed experimental application will be



Fig. 6. Line spread function obtained from 100 ms x-ray radiographs of a x-ray opaque 50 μm thick tungsten knife edge. The x-ray source used was an x-ray tube with a copper anode and a 50 μm thick nickel filter operated at 14 kV and 0.7 mA. Approximate pixel borders are shown with dashed lines.

minimal. Dose testing of the un-bumped ASIC indicates that damage to the CMOS is recoverable by annealing.

TABLE I DETECTOR SPECIFICATION SUMMARY

Pixel Size	$110\mu\mathrm{m} imes110\mu\mathrm{m}$	
Array Size	Single ASIC:	185×194
	Tiled Detector (phase 1):	758 imes 758
	Tiled Detector (phase 2):	1516×1516
Frame Rate	120 Hz in operation at LCLS	
Pixel Saturation	2700 8-keV x-rays (Low-Gain)	
	350 8-keV x-rays (High-Gain)	
Quantum Efficiency	0.97 8-keV x-rays	
	0.89 12-keV x-rays	
	0.48 18-keV x-rays	
Signal-to-Noise Ratio	7 for 8-keV x-ray (High-Gain)	
(rms)	2 for 8-keV x-ray (Low-Gain)	

VI. CONCLUSION

Detector development for new experiments like coherent xray imaging (CXI) has many challenges. Some of these challenges are foreseen and defined in the specifications outlined at the beginning of the project. The detector ASIC we have designed and tested has shown that it is capable of meeting these specifications.

This detector is, beyond an answer to the requirements of one experiment, a template for further detector development. In-pixel digitization, for instance, is likely an increasing trend in CMOS imaging detectors for x-ray science. A purely digital pixel output has the advantage of simplified readout electronics and avoids pit-falls of high-speed analog multiplexing. Adjustable front-end gain is another feature likely to be used more often in charge integrating detector designs because it effectively increases the dynamic range of the detector. There are other methods for increasing the dynamic range [5], but these often limit instantaneous count rates to levels that are incompatible with new, brighter x-ray light sources being developed.

The measurements of charge sharing demonstrates an important advantage of charge integrating detectors that is often lost with counting detectors. This advantage is complete measurement of deposited charge independent of the location of x-ray conversion with respect to pixel borders. When using a detector in the realm where loss of charge through recombination is small, the measurement of charge collected by an integrating front-end is a direct measurement of the xray energy absorbed in the detector. In contrast, detectors that count photons based on pulse shape analysis using discrimination levels are hindered by count-rate limitations and charge sharing between pixels. At very high count-rates like those anticipated in many XFEL experiments, photon counting is not possible.

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