Fast large-area spectroscopic and imaging CCD detectors for X-ray astronomy with eROSITA and for exploration of the nanocosmos

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ABSTRACT

A pnCCD detector fulfils all typical requirement specifications to an X-ray detector optimally: The energy of the X-ray photon is precisely measured, incidence position is determined even more accurate than the pixel size, and the arrival time of the photon is very well defined by the high frame rate due to complete parallel signal processing. The probability for detection of an X-ray photon is from 0.3 keV to 10 keV close to 100% and homogeneous over the image area.

Such a detector has been developed for application in X-ray astronomy. The XMM-Newton space observatory is already equipped with a pnCCD camera which performs since commissioning in 2000 till this day excellent measurements. For the upcoming eROSITA telescope on the Spectrum-Roentgen-Gamma satellite, an advanced pnCCD detector system is presently developed. Seven pnCCD cameras are placed in the foci of seven X-ray mirror systems researching the X-ray sky during a mission time of 5 years.

For ground based instrumentation the X-ray fluxes can be extremely high, as it is the case in X-ray free electron lasers (XFELs). The evolving XFELs will make it possible to capture three-dimensional images of the nanocosmos. Here the focus is set on the measurement of X-ray intensities instead of spectroscopy, i.e. the number of monochromatic photons per pixel (up to > 1000 photons) is counted at very high frame rates (> 100/s).

Both projects have again in common the request for large image areas: in case of eROSITA seven times an image area of 8 cm^2 and for the XFEL experiment at LCLS we provide in a first step a 59 cm^2 large image area. In a second step it will be enlarged to even 236 cm^2. We performed recently promising tests with the prototype detectors. Therefore we started the production of the final devices for both applications in the MPI semiconductor laboratory.

Keywords: eROSITA, LCLS, pnCCD, Spectrum-Roentgen-Gamma, XFEL, X-ray detector.

1. INTRODUCTION

A pnCCD is a special type of charge coupled device (CCD) originally developed for spectroscopy and imaging of X-ray photons. The XMM-Newton satellite of the European Space Agency (ESA) launched in 1999 is equipped with a pnCCD.[1] The 6 cm x 6 cm large image area of the pnCCD is read out with a frame rate of nearly 14 images per second and spectroscopy is permitted at a read noise level of 5 electrons rms. The large pixel size of 150 µm x 150 µm determines roughly the spatial resolution of the X-ray CCD, which has a format of 384 x 400 pixels.

Based on this concept, we developed various advanced pnCCD types for diverse applications. Here we introduce two types of pnCCDs, which have in common a large format, the pixel size of 75 µm x 75 µm, and the application for detection of X-ray photons with high time resolution. However, the requirements for the detectors are quite different in

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terms of X-ray photon flux, signal processing time, energy resolution, geometry, operation temperature and radiation hardness.

One type of pnCCD we develop for the meanwhile approved X-ray astronomy project eROSITA (extended Roentgen Survey with an Imaging Telescope Array)[2]. The X-ray telescope will be accommodated aboard the new Spectrum-Roentgen-Gamma[3] satellite. It consists of seven parallel oriented mirror modules (Wolter-I optics) each having its own pnCCD camera in the focus. One main scientific goal is to perform an imaging all-sky survey up to an X-ray energy of 10 keV with unprecedented spectral and angular resolution. Another primary objective is the investigation of the nature of dark energy and dark matter by mapping out the large-scale structures in Universe by means of the observation of cluster of galaxies. Finally, eROSITA will act as a pathfinder for the next large X-ray observatory XEUS[4, 5]. The satellite launch is planned for the year 2011. The observation time of eROSITA including the all-sky survey as well as the pointed observations will be in total about 5 years.

Another type of pnCCD is produced as detector for the evolving X-ray free electron lasers, a new generation of synchrotron light sources. XFEL facilities provide pulses of coherent X-ray light of high brilliance. The pulse rate is high and the pulse duration short (in the order of 100 fs). For example, the LCLS XFEL will operate with a constant pulse repetition rate of 120 Hz. XFELs will open up entirely new possibilities for experimentation, such as to film chemical reactions, map the atomic details of molecules, and capture three-dimensional images of the nanocosmos. The XFEL pulse is so intense that for example a single particle is destroyed after the pulse. Therefore, from the X-ray diffraction pattern measured during the pulse, the image of the particle has to be calculated.

The LCLS (Linac Coherent Light Source) XFEL at SLAC in Menlo Park, USA, and the European XFEL facility in Hamburg, Germany, are presently set up and will be operational (i.e. first beam) in 2009 and 2013 respectively. These XFEL facilities are supposed to deliver focused mono-energetic X-ray pulses from below 0.3 keV up to 24 keV. At DESY in Hamburg a FEL in the very soft X-ray region (90 eV up to 200 eV) is already in operation, the FLASH (Free electron LASer in Hamburg) facility. At FLASH we performed recently first test measurements with a pnCCD, which was actually developed as prototype for eROSITA.

2. PNCCD DETECTOR FOR EROSITA

The eROSITA X-ray telescope will be equipped with seven independent and identical pnCCD X-ray cameras. We decided recently to increase the image area of the CCD from 256 x 256 pixels to 384 x 384 pixels for the purpose of a higher X-ray photon grasp (i.e. effective area × field of view). With an unchanged pixel size of 75 µm x 75 µm the image area is then 28.8 mm x 28.8 mm large, corresponding to a field of view (FoV) with a diameter of one degree. The other key parameters of the detector remain the same: high energy resolution (close to the theoretical limit given by Fano noise) in the energy region of interest from 0.3 keV to 10 keV in combination with a quantum efficiency of at least 90% [6]. The read noise of the pnCCD detector expressed as equivalent noise charge (ENC) was improved to 2 electrons rms. The time resolution will be kept up at 50 ms, although the number of pixels readouts was increased by a factor of 2.25 due to the larger CCD format. This is possible because readout of the image needs only a fraction of the 50 ms period. The remaining time the CAMEX (CMOS Amplifier and MultiplEXer) readout chip is switched in standby mode to minimize the heat dissipation to the focal plane CCD. By this measure we will achieve a CCD temperature of -80°C on the satellite. The low temperature is necessary to maintain the low-noise performance of the detector over the mission time of five years in spite of the proton environment of space and the resulting radiation damage.

The pnCCD is a 3-phase, back-illuminated charge coupled device with fully depleted chip thickness of 450 µm. The number of generated signal electrons is proportional to the energy of the X-ray photon absorbed in the CCD. The signal charges are stored in the pixels and transferred within the channels to the anodes. In frame store (or frame transfer) mode the image is transferred rapidly to the frame store section with downsized pixels of 51 µm x 75 µm. In the frame store area, which is shielded against X-ray photons, the charges in the pixels are read out row by row, i.e. simultaneously for the 384 channels. This is possible because all channels are equipped with an anode and a JFET for on-chip amplification. A bond wire connects the source of each transistor to the input of a signal processor channel of the CAMEX. The CAMEX ASIC allows amplification and shaping of 128 signals, i.e. of 128 channels, simultaneously.

We use thus three CAMEX chips for the readout of each eROSITA pnCCD detector (see Figure 1). For more details about the pnCCD and the CAMEX readout ASIC, see e.g. ref. 6.

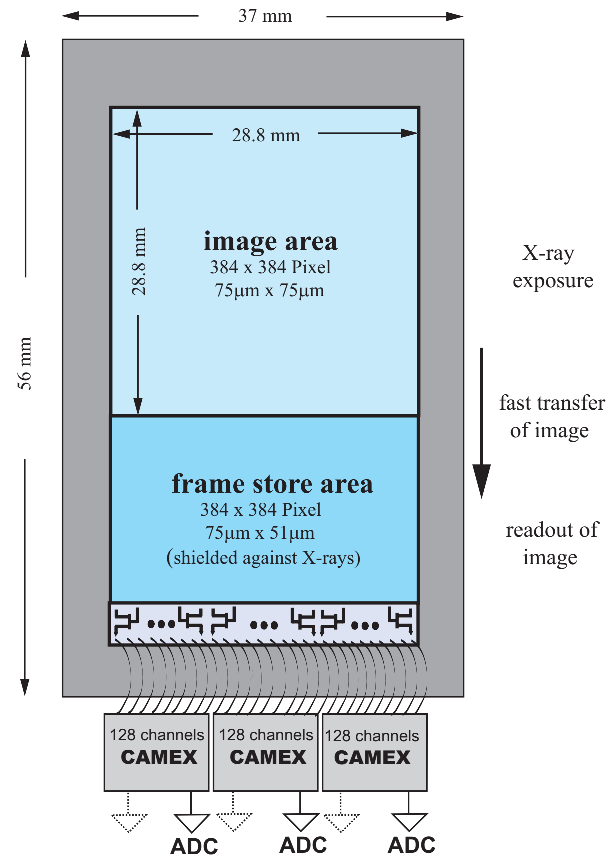

Figure 1: Schematics of the redesigned eROSITA pnCCD. The image area of 28.8 mm x 28.8 mm is subdivided into 384 x 384 pixels with a size of 75 µm x 75 µm. The pixel size in the frame store is downsized to 51 µm x 75 µm. The whole chip size amounts to 56 mm x 37 mm.
Three 128-channel VLSI JFET-CMOS CAMEX chips are employed for the simultaneous readout of the 384 pixel signals per row. The signals of the 128 channels are serialized to one CAMEX output. Only one of the two existing CAMEX outputs is used due to the fact that the readout time does not limit the time resolution of the detector because it amounts to less than 20 % of the exposure time. However, the complexity would increase by doubling the number of output nodes and subsequent electronic chains.

Detector wafers with the eROSITA pnCCDs described above, are presently in production (see Figure 2). Our concept of full chip depletion requires double-sided polished wafers because of processing on both surfaces[6]. We deposit a light filter on the photon entrance window of the chip. It is composed of a SiO_2, Si_3N_4 and Al layer stack. The filter is necessary in space to suppress optical and UV light, which is focused by the telescope onto the detector like X-ray photons. We have to avoid this interference for the purpose of most accurate spectroscopy.

Concerning energy resolution, eROSITA demands from the pnCCD detector most accurate measurement of the energy of the X-ray photons. This requires transfer and readout of the complete generated signal charge at ultra low-noise level. For the purpose of spectroscopy, it is required to collect at most one X-ray photon per pixel. This condition is met by the high frame rate of 20 images per second and the relatively low photon fluxes in X-ray astronomy, although the collection area and the angular resolution of the X-ray mirrors are very high[2]. Optimum energy resolution of the detector needs a sufficiently low operating temperature to avoid any noise contribution by dark current. If we take into account radiation damage caused by protons in space, we aim for an operating temperature of -80°C. In combination with shielding of the CCD chip, this is the only protective measure against radiation damage.

Another special constraint for the CCD module is its durability against the vibrational loading of the satellite launch. Having also regard to the limited cooling power on the satellite, an elaborate design of the detector module including frontend electronics was developed. The first approach is shown in Figure 3. An additional difference to ground based applications is the missing accessibility to the CCD detector except for a few programmable settings in flight.

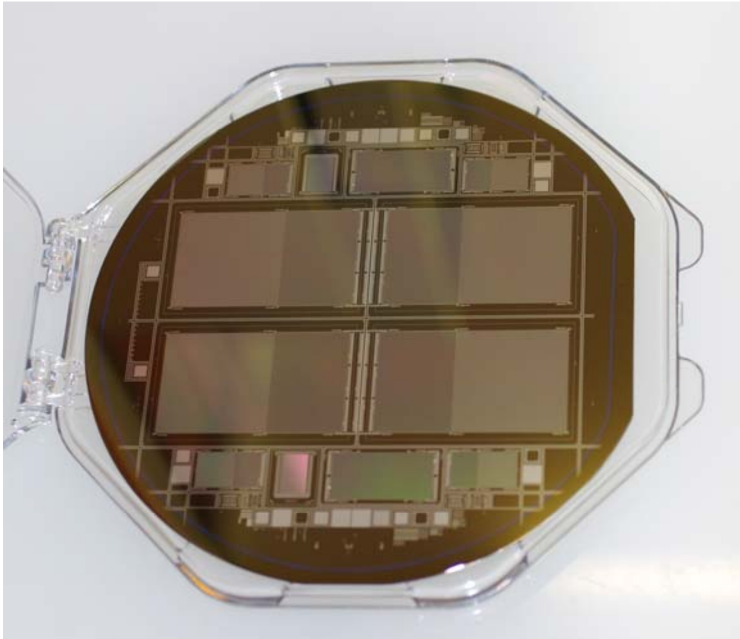

Figure 2: High purity silicon detector wafer containing four large eROSITA pnCCDs plus additional small CCDs and test structures. These CCDs are oriented the way that the frame store area and the on-chip electronics are placed in the center of the 150 mm large silicon wafer.

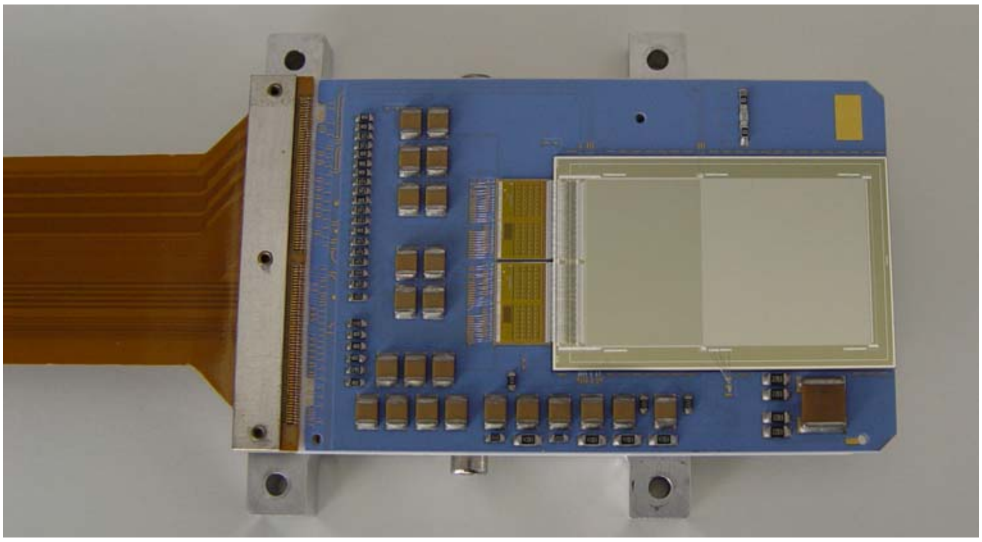

Figure 3: Prototype pnCCD detector of the eROSITA flight cameras with a 256 x 256 pixel CCD. The type of board is similar to that used in the laboratory setup but instead of multi-pin connectors, a flexible lead (left hand side of figure) is used. The detector assembly consists mainly of a multi-layer printed circuit board (PCB), two CAMEX chips and the pnCCD. The PCB was made in hybrid circuit technology on a ceramic substrate (Al_2O_3). The CCD and the ASICs were mounted and wire bonded onto this PCB. The thermal and mechanical interface is located on the back side of the module. The flight CCD has by a factor of 2.25 more pixels and will be read out by three instead of two CAMEX ASICs.

3. PNCCD DETECTOR FOR XFEL EXPERIMENTS

The pnCCDs developed for XFEL experiments have an even larger format than the eROSITA CCDs. The detector for LCLS is in the first phase composed of two CCDs with 1024 x 512 pixels each (see Figure 4). This improves the yield of the CCD production at the cost of an insensitive gap of about 1 mm between the two CCD chips of the detector. The pixel size is the same as for eROSITA, 75 µm x 75 µm. The image area of the CCD chip has thus a size of 59 cm^2. Commissioning of this high-speed, large-area detector is planned for the year 2009. The implementation of readout of the image in two directions (split frame mode) reduces the readout time by a factor of two for the price of doubling the readout electronics. Eight 128-channel CAMEX chips are thus in use per CCD chip and sixteen ASICS per detector respectively. In contrast to eROSITA we employ both output nodes of the CAMEX ASIC for a faster readout. In this case twice the number of ADCs has to be provided. Therefore the electronics system is equipped with 32 ADCs running at 10 MHz each with a resolution of 14 bit. A description and test results of a first fast pnCCD detector system are given in ref. **7**.

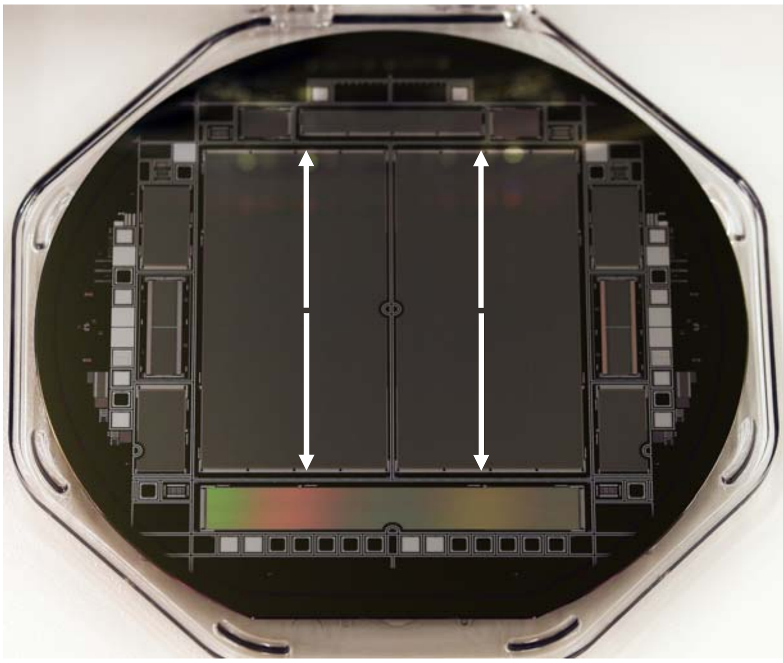

Figure 4: Wafer with two 1024 x 512 pixel pnCCDs as designed for XFEL applications. The two chips are cut out of the wafer and build up a 1024 x 1024 pixel large CCD detector with a hole in the centre for the primary X-ray beam. Theses CCDs are read out in two directions (as indicated by the arrows), the upper half of the pixels is transferred and read out upward and the lower one downward.

The application of the pnCCD as XFEL detector differs regarding energy resolution from the eROSITA project by the fact that the energy of the X-ray photons is precisely known. However the photon energy depends on the experiment and can have a value between 0.3 keV and 24 keV. The task in this application is to measure the number of photons per pixel and frame. The important capability of the detector is to distinguish one photon per pixel from no photon over the full energy range. Equally essential is a large dynamic range of the detector system allowing for photon intensity measurements of up to 10^3 photons per pixel with a precision of $N^{½}$, with N being the number of photons.

The relaxed requirement for energy measurement is necessary to achieve the readout of a 1024 x 1024 pixel large pnCCD image at a high frame rate of 250 images per second. The CCD is operated in full frame mode, not in frame store mode, because the CCD readout is synchronized with the XFEL X-ray photon pulses. The highest number of photons can be measured if the CAMEX is operated in lowest gain. In this configuration we achieve a maximum energy of a few MeV per pixel and a read noise of less than 25 electrons rms. If the system is operated with highest gain, which limits the total energy to a few keV per pixel, the system noise is about 2-3 electrons (rms). Preferred operation temperature is -20°C but also higher temperatures up to room temperature are considered.

At X-ray energies above one keV the quantum efficiency of the detector is just determined by the absorption probability of the photon in the thickness of the sensitive detector volume. Due to the concept of the pnCCD that the whole chip thickness of 450 µm is fully depleted, we achieve high quantum efficiency also for high X-ray energies. At the maximum X-ray photon energy of 24 keV in XFEL experiments we obtain still a quantum efficiency of 20%. The high charge storage and handling capacity per pixel of 10^5 electrons will be upgraded for the pnCCDs developed for XFEL to 1×10^6 electrons per pixel by additional implants in the pixels. Thus it will be possible to store the signal charges of more than 1000 X-ray photons per pixel. The XFEL detector wafers (see Figure 4) are presently in production as the eROSITA CCD wafers. The central region of the XFEL CCD detector features a hole with 3 mm diameter that will be cut with a laser in the silicon for passage of the not diffracted X-ray photons of the pulses.

In a second phase, a 1024 x 1024 pixel large pnCCD will be produced with readout along only one side, i.e. each transfer channel comprises then 1024 pixels. The image is then read out in 8 ms instead of 4 ms permitting a frame rate of 125 images / s. That way this system is three-side buttable and can be extended to a 2048 x 2048 pixel array with an image area of 236 cm^2. Such a system is planned for the year 2011.

For XFEL purposes, a development program has started in spring 2007 in the frame of the Center for Free Electron Laser science (CFEL), a joint effort of the Max-Planck Society, DESY, and the University of Hamburg.

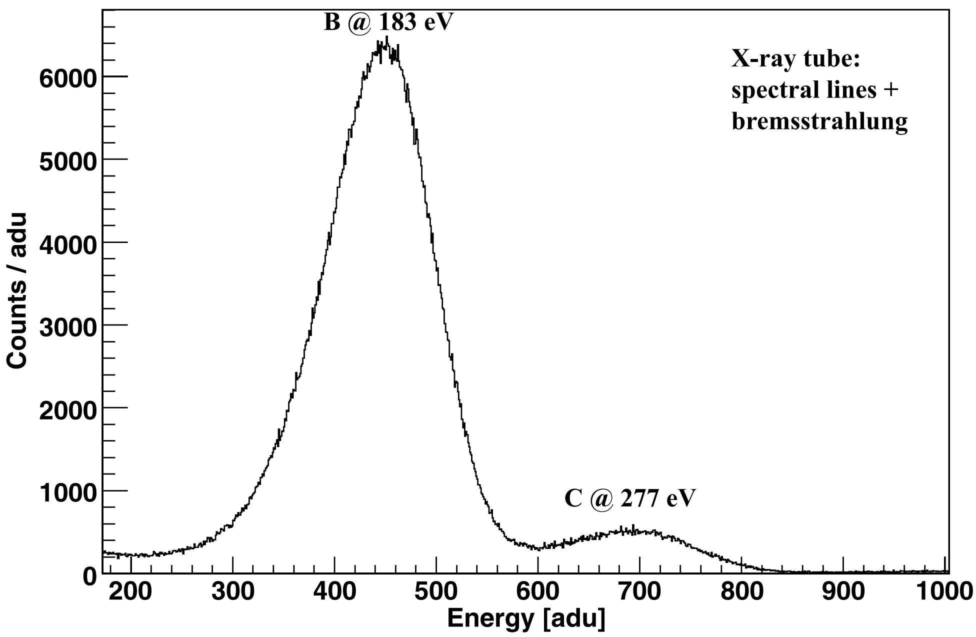

Figure 5: Spectrum of boron line at 183 eV and carbon line at 277 eV measured with a pnCCD detector. The lines were generated by an X-ray tube. The CCD of eROSITA prototype is equipped with a light filter on the photon entrance window and was operated in highest gain mode for this special measurement. We determined a FWHM of 51 eV for the boron line.

4. RECENT X-RAY MEASUREMENTS WITH PNCCD DETECTORS

We have already produced and tested pnCCDs with 256 x 256 pixels in the image area, which are apart from the format like the eROSITA pnCCDs. They are already equipped with the light filter as required for eROSITA. We call them therefore eROSITA prototype pnCCDs. The signals at the anodes are amplified by pnCCD on-chip transistors which are operated in source follower mode. The CAMEX readout ASIC is programmable by internal registers, especially the number of signal samplings and the gain level. In case of ultra low-noise performance, as demanded by eROSITA, we select 8-fold correlated double sampling of the signals and a high gain of the CAMEX permitting spectroscopy of up to 12 keV. If high-speed performance and a maximum dynamic range are required, we choose only single correlated double sampling and select a low gain of the signal processing ASIC. The CAMEX settings can be chosen appropriate to the particular application.

The continuance of the excellent energy resolution of the pnCCD in the very soft X-ray energy region is demonstrated by spectroscopic measurements of the boron fluorescence line at 183 eV (see Figure 5). The full width at half maximum (FWHM) of the energy spectrum was determined to 51 eV. A standard laboratory pnCCD detector module with control electronics and data acquisition system as described in ref. 6 was used for the tests. Spectroscopy of lines from the very soft X-ray region is challenging because the electron-hole pairs are generated close to the surface of the silicon detector. Nevertheless nearly all signal electrons which are generated by a boron X-ray photon, are obviously collected in the pixels. This requires fast separation of the generated electrons and holes by a sufficiently high electric drift field and an extreme low trap density even at the Si-SiO_2 interface. A clear separation of the boron spectrum from the noise peak needs furthermore ultra low-noise readout. The total read noise here is 2 electrons rms. Please note that the energy of the boron line is already lower than the lower limit of 0.3 keV of the nominal eROSITA energy band. The excellent low X-ray energy performance will potentially open completely new fields of applications for pnCCDs.

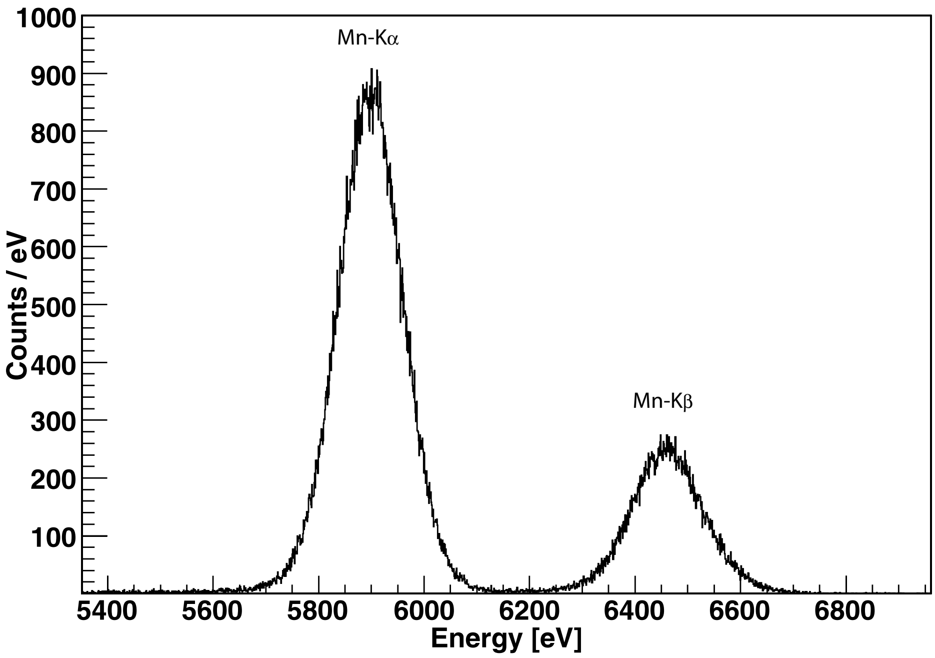

Figure 6: Fe55 spectrum measured with a prototype of the pnCCD flight detector, which is shown in Figure 3. The FWHM of the Mn-Kα line is 139 eV. The energy resolution of the prototype flight detector is similar to that of the modules designed and used for tests in the laboratory.

A special design of the detector is necessary for eROSITA aboard the Spectrum-Roentgen-Gamma satellite as explained above. Figure 3 shows the first prototype of the eROSITA CCD-module with 256 x 256 pixel large image area. A flex lead connects the CCD module to the camera electronics. Electric components which are critical for optimum detector performance are integrated as close as possible to the module. For example the digital pulses are converted on the flex lead into analog CCD clock pulses for optimum charge transfer efficiency. Analog output buffers, one per CAMEX, are also accommodated on the flex lead. For thermal reasons we have to arrange these active and heat dissipating components on the "warm" side of the flex lead which is separated by the length of the flex lead from the cold CCD module.

This module was recently tested for the first time. We obtained a read noise of 2.3 electrons ENC and a FWHM of the Mn-Kα line (5894 eV) of 139 eV. A Fe55 spectrum measured with this module is shown in Figure 6. The results of the experimental test verify our detector concept conceived for eROSITA. The module overcame the vibration and thermal-vacuum tests. The electric performance tests completed the verification of our detector concept for eROSITA. We will thus adapt in the next step the design of the detector module to the larger format eROSITA flight pnCCD.

Operational experience for future XFEL experiments was gained with existing pnCCD detectors in measurements at the BESSY synchrotron and the FLASH light source. Figure 7 shows a spectrum of photons with energy of 90 eV, measured at the FLASH free electron laser. Further information about the measurements including images is presented in ref. 8.

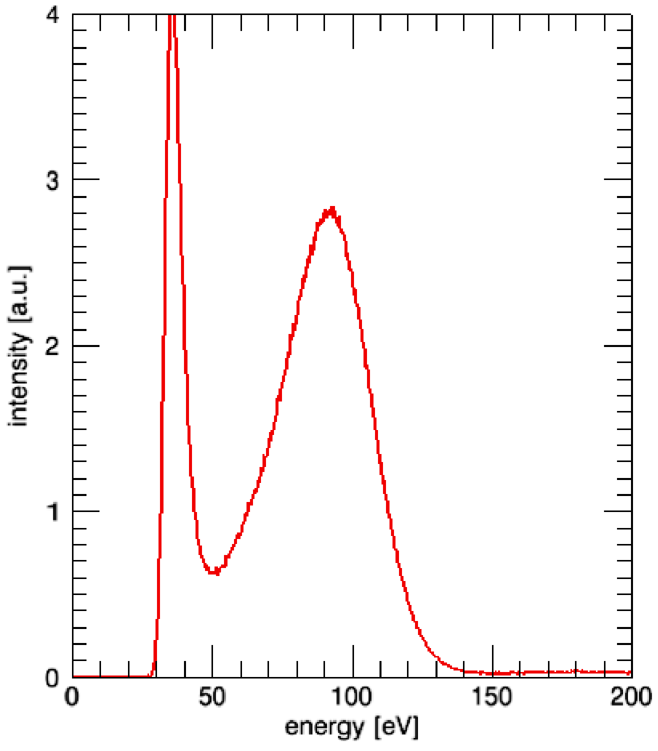

Figure 7: Spectrum of mono-energetic 90 eV photons generated by the FLASH free electron laser measured with a pnCCD. The signal peak is clearly separated from noise and higher harmonics of the laser. A FWHM of 39 eV was determined for the 90 eV peak.

5. SUMMARY AND OUTLOOK

Two designs of pnCCD detectors were presented, one for the eROSITA X-ray space telescope and a second for X-ray free electron laser experiments in near future. Several experiments with prototype detectors showed the feasibility and performance prospects. In both applications, we measure the energy of X-ray photons and take images with fast large-area pnCCD detectors. However, the requirements for X-ray astronomy on a satellite and for fast two-dimensional imaging with high-intensity coherent light of an XFEL differ considerably in several performance features. The key features of both detector types are summarized in Table 1. The appropriate CCD devices are presently in production. During the next four years, both types of fast large-area pnCCD detectors have to be built up, tested and calibrated.

Table 1: Key features of the pnCCD detectors developed for eROSITA and XFEL experiments.

Parameter	**eROSITA**	**XFEL**
Format	384 x 384 pixels (image area) + + 384 x 384 pixels (frame store)	1024 x 1024 pixels (phase I) 2048 x 2048 pixels (phase II)
Pixel size	75 x 75 μm^2 (image area) and 51 x 75 μm^2 (frame store)	75 x 75 μm^2
Image area	8.3 cm^2 per detector 58 cm^2 total eROSITA	59 cm^2 (phase I) 236 cm^2 (phase II)
Energy range	0.3 keV - 10 keV	0.3 keV - 24 keV
Depletion depth	450 µm	450 µm
Quantum efficiency	≥ 90 % from 0.3 keV - 11 keV (without optical filter)	≥ 90% 0.3 keV -11 keV; 64% at 15 keV; 35% at 20 keV; 20% at 24 keV
Photon flux (typ.)	0 or 1 / (pixel · frame)	0 … 10^3 / (pixel · frame)
Charge handling capacity	10^5 electrons / pixel	1 x 10^6 electrons / pixel
Operation temperature	-80°C (radiation damage in space)	-20°C preferred (room temperature possible)
Read noise	2 e^- ENC	≤ 25 e^- ENC
Energy resolution (20 images/s, T=-70°C)	FWHM(90 eV) = 39 eV FWHM(183 eV)= 51 eV FWHM(5.9 keV)= 139 eV	Resolution of number of photons in pixel
Readout time	< 26 µs/row (=384 pixels) or < 10 ms/8.3 cm^2 image	7.8 µs/row (= 1024 x 2, 4096 pix. in phase I, II) 4 ms/59 cm^2 (phase I) 8 ms/236 cm^2 (phase II)
Pixel readout rate	> 15 Mpix/s (during readout phase)	263 Mpix/s (phase I), 525 Mpix/s (phase II)
Frame rate	20 / s (due to thermal budget)	250 / s (phase I) and 125 / s (phase II)
Operating mode	frame store (frame transfer)	full frame
Fast transfer	200 µs / 8.3 cm^2 image	n.a.
'Out of time' event occur.	0.4%	0% (events synchronized with readout)
Schedule	satellite launch: 2011	phase I: 2009; phase II: 2011

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