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The use of CCDs and EM-CCDs for future soft X-ray Spectrometers

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ABSTRACT

CCDs have been used on several successful X-ray space missions including high resolution soft X-ray spectrometers, such as the Reflection Grating Spectrometer on XMM-Newton[1] and the LETG and HETG on Chandra[2]. These instruments had a resolving power of ($\frac{E}{\Delta E}$) ~300; however, with new technology this can be improved allowing resolution to the thermal limit. In the soft X-ray band (200 eV to 10 keV) a resolution of around 3000 is required resolve all of the possible absorption and emission features. Through the development of instruments for the OP-XGS on IXO[3] and the WHIMEx explorer mission[4] it has been shown that an instrument capable of this resolution on a spacecraft is possible. CCDs are the ideal detector for use in detection of X-rays at this energy as they provide positional information allowing a high level of spatial resolution and their inherent energy resolution allowing diffracted orders to be separated. This paper will investigate the use of CCDs and possible use of EM-CCDs in soft X-ray spectroscopy. The multiplication of signal in the charge domain can increase the detectability of low energy photons, improving the Signal-to-Noise Ratio. Multiplication gain has been shown to degrade the resolution of a device as described by the Modified Fano Factor[5], so this has to be taken into account in instrument design when overlapping spectral orders are needed to achieved the necessary resolution. The use of optical filters on the CCDs and their effect on quantum efficiency at soft X-ray energies is discussed together with possible improvements to existing technology.

Keywords: CCD, EM-CCD, Spectrometer, Soft X-ray, Fano Factor, Modified Fano Factor, Optical filters

1. INTRODUCTION

CCDs have been widely used in X-ray space missions since they were first flown on the Advanced Satellite for Cosmology and Astronomy (ASCA) by Japan in 1993[6]. Since this mission, the ability of a CCD to image incident photons with high spatial and spectral resolution and with a high Quantum Efficiency (QE), has led to CCDs being used on high resolution X-ray spectrometers such as the Reflection Grating Spectrometer (RGS) on XMM-Newton[1] and the ASIC on Chandra[2]. With the drive towards ever increasing effective area and resolution, the use of CCDs on the focal plane array for dispersive spectrometers is forced to develop. Devices that can be deep depleted have been developed, giving an increase in the spectral resolution performance possible with CCDs[7] and, conversely, centroiding algorithms have been developed to produce sub-pixel spatial resolution through the re-construction of split events[8,9].

A further development in soft X-ray detection has been the use of EM-CCDs to allow better detection efficiency of low energy X-ray photons. Through the use of internal gain, the readout noise of the system, which can be dominant at low energies, is suppressed allowing the effective detection of X-ray photons at sub 300 eV energies[10]. Also, as the position of the interaction of the photon determines the energy, only part of the charge-cloud generated by the X-ray needs to be detected. With sufficient cooling, a charge packet of a few electrons can be detected above the noise floor through the use of multiplication gain allowing the extension of the bandpass to much lower energies. The readout noise suppression will also allow a much faster readout of the CCD; therefore, higher flux sources of X-rays can be observed without saturation of the device.

Dispersive spectrometers use overlapping orders to achieve a high efficiency from the grating optics; hence, the detectors on the focal plane array are required to distinguish between these orders to determine the energy of the incident photon[11]. Degradation of the spectral resolution of an EM-CCD, either due to the charge being split across several pixels or due to

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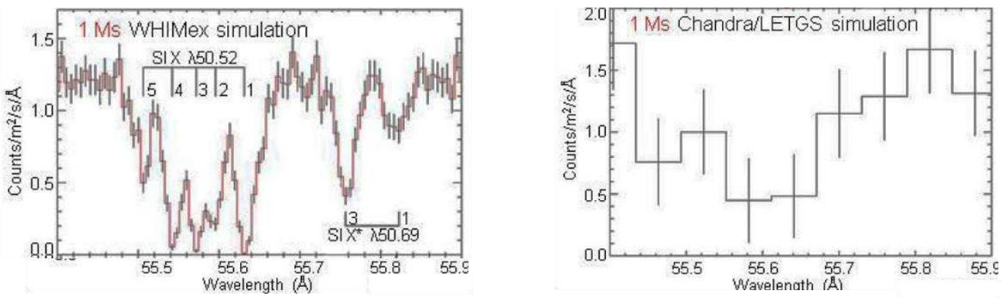
the additional noise from multiplication gain, can cause the detector to fail to resolve the overlapping orders; therefore, this effect has to be carefully analysed when designing a spectrometer.

2. DISPERSIVE X-RAY SPECTROMETERS

X-ray spectrometers that use gratings and the spatial resolution of the detectors on the focal plane have been used on XMM-Newton[1] and Chandra[2]. The dispersion from the grating separates out different X-ray energies across the focal plane and the resolution achieved by the instrument is dependent on the level of dispersion that can be achieved from the grating (a function of the number of grooves on each grating) and the distance between the grating and the focal plane (the throw). Producing an instrument with a high resolution is attractive as it allows narrower features to be identified in emission and absorption spectra, Figure 1. The ability to detect narrow features allows more detailed analysis of X-ray sources to be made, increasing our understanding of these objects.

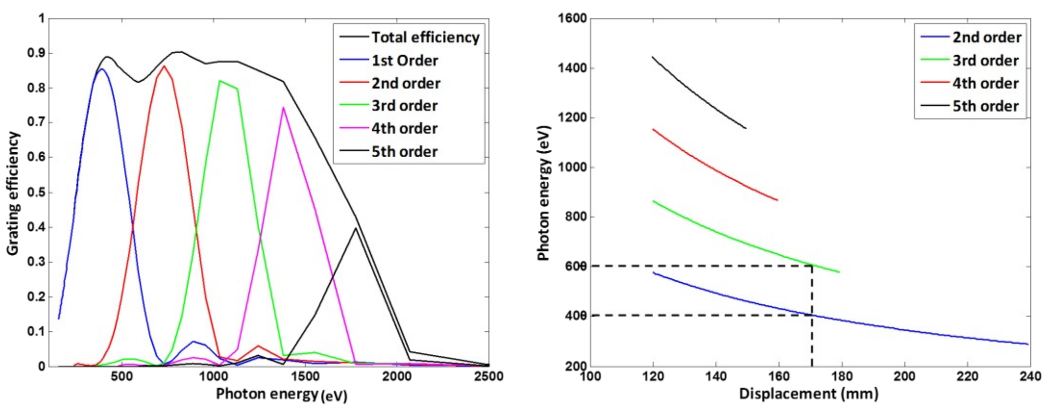


(a) (b)

Figure 1: Simulated observations with WHIMEx (a) and Chandra (b) of the same outflow feature showing the importance of high resolution[12]. The WHIMEx simulation is at a higher resolution (4000) than Chandra (300).

2.1. Grating efficiency

The efficiency of a grating is a measure of the proportion of photons incident onto the grating that are then dispersed and fall onto the focal plane. The efficiency of a grating will be optimal at a particular energy for each dispersed order. To get the necessary grating efficiency across the energy range of the instrument, several dispersed orders are used and the sum of all of the orders gives the total efficiency.



(a) (b)

Figure 2: Plots of grating efficiency against energy (a) and the overlapping energies at different orders (b). To achieve the necessary efficiency over the OP-XGS bandpass, multiple order of dispersed photons are used. Multiple orders are required to ensure the OP-XGS achieves its baseline effective area (a). Plot (b) shows at what distance from the zero-order position dispersed X-rays will fall on the camera array. It shows that photons in second and third order at 400 eV and 600 eV respectively will fall at the same point on the focal plane[11].

Figure 2 (a) shows that an efficiency of over 80% can be achieved by a grating across the 300 eV to 1500 eV range using orders 1 through 5; however, a grating will diffract different energy photons in different orders to the same position on the camera array and, as the position that the X-ray is incident on the focal plane determines the energy, this can be problematic to determining the original energy of the X-ray photon Figure 2 (b). With the use of multiple orders, the detectors used in a spectrometer requires a spectral resolution that allows different energy photons to be identified; therefore, a knowledge of which energies will fall at the same position on the focal plane is necessary. With this information a requirement can be put on the spectral resolution of the detector used.

2.2. Spectral resolution requirement

For the OP-XGS the detector is required to resolve photons at 400 eV and 600 eV. By modelling a CCD with near Fano-limited performance, the ability of the device to separate out these two energies can be predicted, Figure 3.

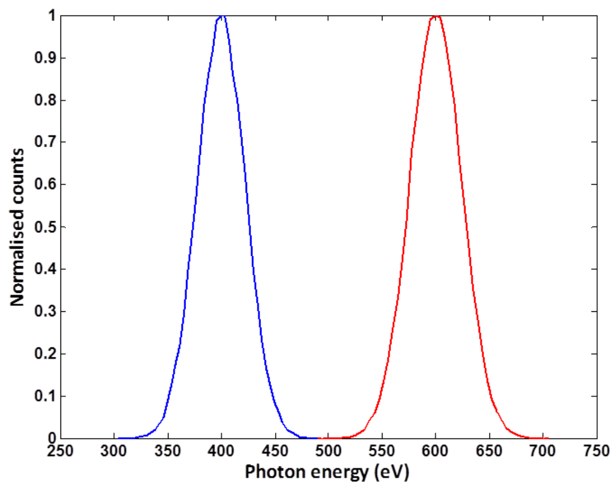


Figure 3: The Fano-limited spectral resolution performance for a CCD detecting 400 eV and 600 eV photons. The simulated X-ray peaks are separate showing that the spectral resolution of the detectors is suitable for the instrument design.

Figure 3 shows that a CCD can be used as the detector for the OP-XGS as it is able to separate out the different diffracted orders. The performance shown is best case, start of life with all X-ray events being collected in single pixels. Some degradation from this performance would be seen in experiment, but the result shows that a CCD is capable of the necessary spectral resolution.

Future spectrometers have also been proposed to continue the trend towards higher resolution X-ray spectroscopy through the Off-Plane X-ray Grating Spectrometer on the International X-ray Observatory[3] and WHIMEx[4]. The remainder of this paper looks at the requirements of a CCD that could be used on an X-ray spectrometer.

3. CAMERA ARRAY CONSIDERATIONS

3.1. Quantum Efficiency

The first consideration for a spectrometer that operates in the soft X-ray band is Quantum Efficiency (QE). It has long been known that the back-illumination of a CCD produces a higher QE over low energies, Figure 4, allowing a much better science performance. However, this does come at a cost to spectral resolution. The incident X-rays generate photo-electrons close to the device surface; therefore, they have a significant amount of silicon to drift through before collection in the buried channel. The thicker the device, the larger the charge cloud becomes and the less likely the charge is to be collected in a single pixel[13]. The formed split event leads to spectral resolution degradation. Split events can be reduced through the back-thinning of the CCD, although this can affect the devices high energy response, or through using a higher resistivity silicon and driving the depleted region to the surface. Despite this potential drop in spectral resolution, the increase in QE makes back-illuminated CCDs the preferred detector for spectrometers working in the soft X-ray energy range[14].

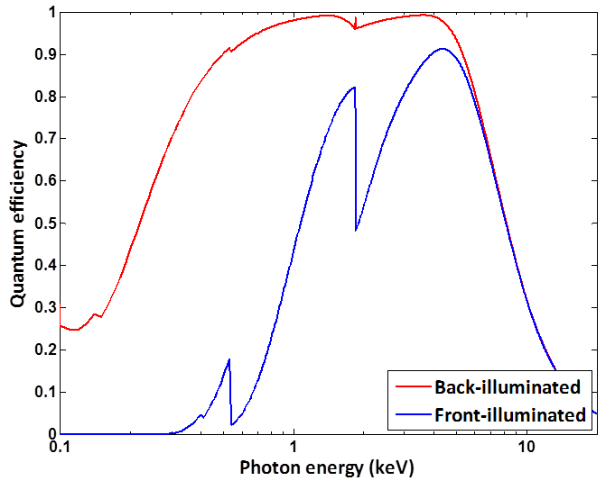


Figure 4: Quantum efficiency plots for modelled front and back-illuminated CCDs over the 0.1 keV to 20 keV energy range.

3.1.1. Stray light tolerance

Spacecraft telescopes will collect optical light as well as X-rays that the CCDs are able to detect. Any optical photons that are detected will lead to an increase in the background of the detector and a reduction in the Signal-to-Noise (S/N) ratio. To counter this affect, space instruments can incorporate aluminium over the detector to make them optically blind. The RGS on XMM-Newton used three different thicknesses of Al depending on the energy of the X-rays that the CCD was aiming to detect, Figure 5 (a). The lower the energy, the large the effect the filter will have on the QE and so the thinner the filter used. Through the use of filters, the QE of the detector falls and this effect is more pronounced at lower X-ray energies, Figure 5 (b). To maximise the CCD QE, the filter used needs to be as thin as possible, but to maximise stray light attenuation the filter used is required to be thick[16].

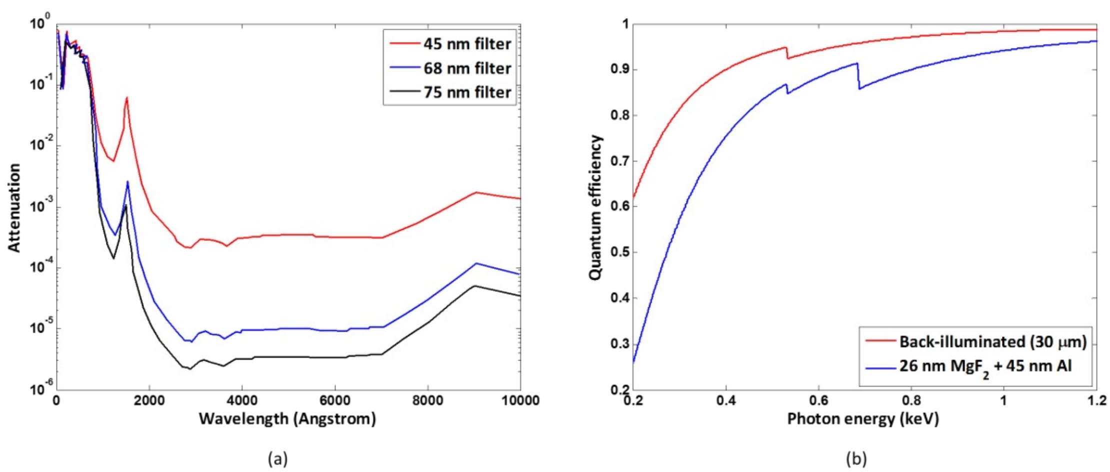


Figure 5: Optical attenuation plots for the three filters used on the CCDs for the RGS on XMM-Newton (a). The reduction in QE through the use of the thinnest filter used on the RGS (b)[15,16].

The stray light tolerance of a detector is strongly dependent on how fast it can be read out. With higher readout speeds a higher stay light flux can be accommodated without degrading S/N; however, an increase in readout speed will also lead to an increase in readout noise. The increasing in readout noise will limit the minimum energy that the instrument will be able to detect above the noise floor unless the noise can be suppressed. The use of EM-CCDs on X-ray spectrometers for readout noise suppression is discussed later in this paper (Section 4.2).

3.2. Detection efficiency

When photons are detected close to the surface of a back-illuminated device, some of the electrons in the charge cloud can be lost in the back-surface generation/recombination centres at the $Si\text{-}SiO_2$ interface[14]. The loss in charge causes the detected X-ray peak to fall at a lower energy on a histogram of events than it should causing inaccuracies in the measured signal and a degradation of spectral resolution. The amount of charge lost to the back surface in a CCD30-11 when tested at the Physikalisch Technische Bundesanstalt (PTB) beamline in BESSY II can be seen in Figure 6.

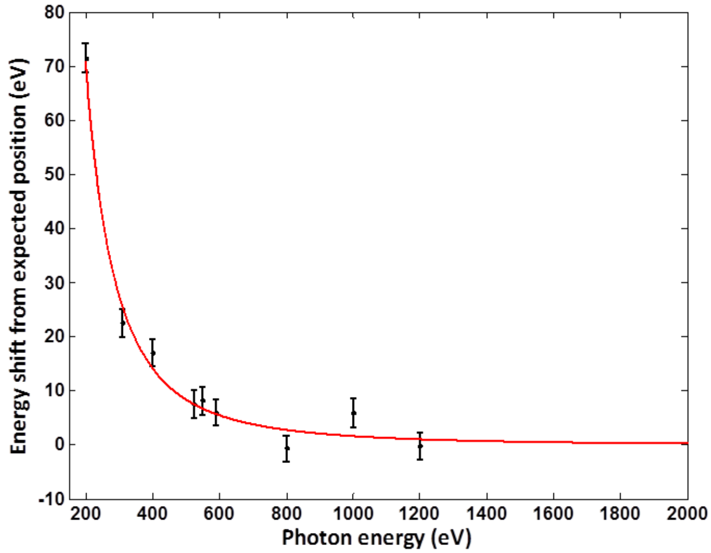


Figure 6: The partial event fraction for a CCD30-11 tested using the PTB beamline at BESSY II across the 150 eV to 1200 eV energy range.

The minimisation of the partial event fraction in a CCD is possible through the optimisation of the back-surface passivation techniques used. By making the dead-layer as thin as possible, a large proportion of the charge loss can be mitigated. Back-surface passivation can be achieved through many techniques including a "UV flood"[17], ion implantation[18], and molecular beam epitaxy (also known as delta doping)[19].

3.3. Spatial resolution

Depending on the design of the instrument either the spectral or spatial resolution can be optimized. For high resolution in a dispersive instrument, the position that the X-ray interaction occurred on the detector should be measurable accurately. Sub-pixel resolution is possible through the use of centroiding algorithms on charge clouds that are split over several pixels. It has been shown that "basic" centre-of-mass algorithms can be used to give interaction positional information to ~3.4 µm accuracy with 1 keV energy X-rays[8,9], Figure 7.

The increase in spatial resolution comes at a cost to the spectral resolution of the CCD. If charge is spread across several pixels, event reconstruction is necessary to collect all of the charge generated by the X-ray interaction[14]. Event reconstruction adds noise to the image, increasing the FWHM of the X-ray peak; therefore, reducing the spectral resolution. Charge splitting can also lead to incomplete charge collection in the image which can cause photo-generated charge to be lost due to the thresholding algorithms used in the data analysis[5]. This will also cause a broadening of the X-peak. Degradation in spectral resolution places a larger energy separation requirement on the instrument than if all of the charge is collected in a single pixel if the device is still going to be able to separate dispersed photons from overlapping orders.

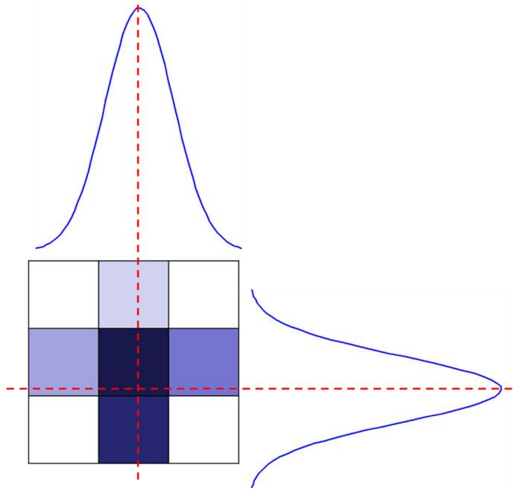


Figure 7: A diagram showing how split events can be used to find the position of interaction in a CCD with sub-pixel accuracy

To maximise the amount of charge that is collected in single pixels the device can be depleted to the back-surface through the use of high resistivity silicon or through the use of large pixels (this can be achieved by using a larger pixel device or by binning the signal "on-chip")[14].

The pixel size, binning and silicon resistivity that is used on a detector is dependent on the specifications that the spectrometer is required to meet. If overlapping orders can be suitably separated then smaller pixels and charge splitting between pixels will offer the highest level of resolution to the instrument; however, with radiation damage effects that are expected in space, the degradation of spectral resolution that would occur due to the maximisation of spectral resolution will become worse as the missions develops.

3.4. Spectral resolution

The spectral resolution of the CCD is required to separate out overlapping orders. It has been shown (Figure 3) that in a Fano-limited case a CCD is able to achieve the spectral resolution required for the OP-XGS on IXO. However, in real conditions many things will degrade the spectral resolution of the system and this could lead to confusion between the X-ray peaks detected, Figure 8. If event splitting is used for sub-pixel photon interaction detection, the partial event fraction is high and the detector is degraded over the course of the mission through radiation damage, overlapping orders may no longer be able to be distinguished using the detectors spectral resolution.

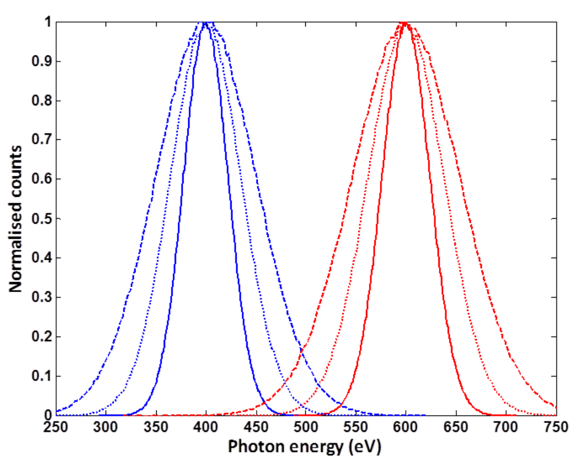


Figure 8: The spectral resolution shown in Figure 3 is degraded to show how peak confusion could occur in the CCD. The curves are for X-ray events that occur in single pixels. Event splitting would lead to a broadening of the peaks through incomplete charge collection or additional noise from event recombination, adding to the confusion between signals.

To avoid X-ray peak confusion, the expected spectral resolution degradation needs to be calculated and the dispersion of the gratings controlled to build in the necessary margin for the detector to reach end-of-life with the desired performance. An increase in dispersion can be achieved through increasing the number of grooves on the grating or by increasing the throw.

4. CCDs vs. EM-CCDs

4.1. CCDs

Charge-Coupled Devices (CCDs) are efficient detectors for soft X-ray spectrometers as they have a high QE over these energy range (>80% between 300 eV and 2000 eV), they can be read out relatively slowly and achieve a low system noise, they can be cooled to reduces dark current, and the use of deep depleted material can minimise the amount of event splitting, maximising the spectral resolution.

CCDs are the workhorse of the X-ray detection community and have been used on many missions since their first use on ASCA[1,2,6] and as a result they have a high Technology Readiness Level (TRL) and are considered reliable. However, to maximise science performance, the CCDs need to have as high a QE as possible. As discussed earlier in this paper, to maximise QE, thin optical light blocking filters are required which means the device has to be read out quickly. A faster readout leads to an increase in readout noise, which will limit the low energy response of the system and so this readout noise needs to be suppressed.

4.2. EM-CCDs

EM-CCDs offer a number of advantages over conventional CCDs in terms of readout noise suppression. EM-CCDs are made by taking a conventional CCD structure and adding a multiplication register to the serial register before the output node[10]. By applying a large electric field to the silicon in the multiplication register extra electrons are added to the charge packet through impact ionization. The increase in the signal before the addition in the readout noise effectively suppresses the readout noise and so smaller signals can be detected in the CCD. The increase in the amount of charge read out for small signals allows the lower energy end of the bandpass to be extended as the increase in low level signal helps move the X-ray photons out of the noise. It can be seen from the dispersed spectrum generated using RGS, Figure 9, that low energy photons come close to the noise floor. With an EM-CCD, the signal readout for these photons would be increased, removing them from the noise floor.

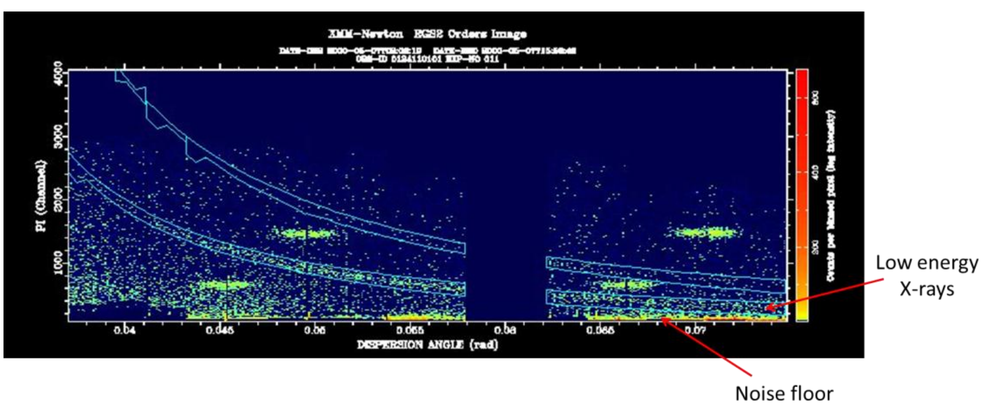


Figure 9: Plot of dispersion angle against energy for the RGS on XMM-Newton with the low energy X-rays position marked in relation to the noise floor[16].

Readout noise is closely related to readout speed. With the increase in pixel frequency the readout noise on a device increases and so the speed that a conventional CCD can be read out at is restricted. With the noise suppression ability of an EM-CCD, the increase in readout noise with increasing pixel frequency has a smaller effect on the noise of the system allowing the device to be readout at a much higher speed for the same increase in readout noise as in a conventional CCD. This higher speed means that the optical stray light tolerance on the system is relaxed, the filters on the devices can be thinner; hence, the CCDs can have a high QE at low energies, improving the potential science yield.

However, multiplication gain is a stochastic process and so the use of gain causes an increase in the noise of the device. The noise is dependent on the amount of gain that is used (for gains of < 10) and has been described by the Modified Fano Factor[5]. The increase in noise causes a degradation of the spectral resolution of the device which can become problematic in a spectrometer if the overlapping orders are not separated by a large enough energy. By using the Fano-limited response shown in Figure 3 and applying the result for Modified Fano Factor for high levels of gain, X-ray peak with multiplication gain related spectral resolution degradation can be produced, Figure 11. The overlap caused by this degradation is shown to be predictable and the effect is well characterised and modelled. By increasing the groove density and throw of the spectrometer the energy between overlapping orders will be increased and the X-ray peaks will no longer overlap.

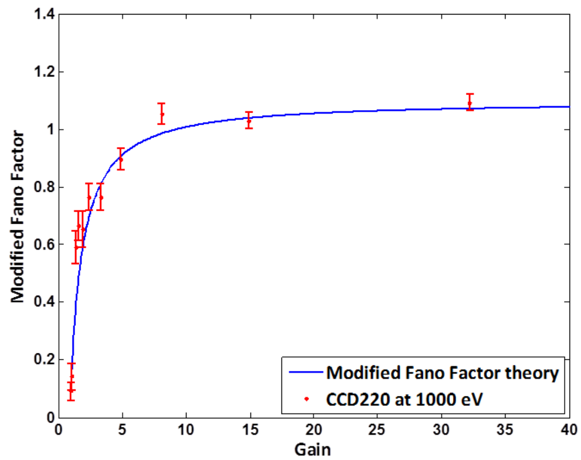


Figure 10: Plot of the Modified Fano Factor with increasing gain using a CCD220 at 1000 eV[20].

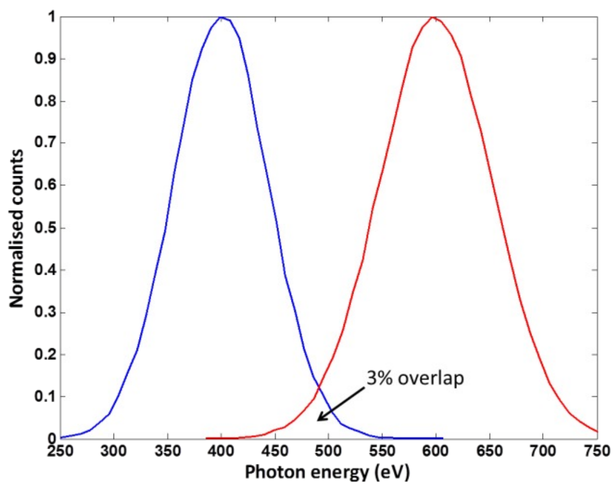


Figure 11: The Modified Fano Factor limited spectral resolution performance for an EM-CCD detecting 400 eV and 600 eV photons with a high level of gain. The simulated X-ray peaks do overlap showing that the spectral resolution of the detectors is not suitable for the instrument design.

5. CONCLUSIONS

When choosing an ideal detector for a high resolution soft X-ray spectrometer several factors have to be taken into account and balanced to produce the highest quality instrument possible.

The major constraint on what decisions you make about the detector stem from the frame rate required. If you are able to have a high frame rate, not only can brighter sources be observed without pile-up and saturation, but the stray light tolerance on the detector is relaxed allowing thinner optical blocking filters to be used. In turn, thinner filters increase the QE of the detector at the lowest X-ray energies of the instrument bandpass increasing the possible science yield. However, a CCD running faster will also have an increase in readout noise.

Using an EM-CCD allows the use of internal gain in the multiplication register to suppress the readout noise and the device can be run faster without compromising the read noise floor. The multiplication of the signal in the charge packet before it is read out moves lower energy photon events out of the noise, causing them to be more easily detectable. The increased ability to detect low energy photons will allow the bandpass of the instrument to be increased to lower energies (to include the carbon K-shell for example at 277 eV[15]) potentially increasing the possible science that the instrument could achieve.

Multiplication gain causes a broadening of the detected X-ray peak due to the stochastic nature of the gain process and this leads to degradation in spectral resolution. However, extensive work has been completed to model and characterise this effect as the Modified Fano Factor. The factor allows predictions to be made about the degradation and, thought the manipulation of throw and grating groove density, the affect can be compensated for. EM-CCDs are still currently considered to have a low TRL, but with further testing in space-like environments, this can be improved.

The CCD used on a soft X-ray spectrometer will have to be back-illuminated to provide the necessary QE across the energy range and the surface is required to be passivated with the thinnest dead-layer possible to maximise detection efficiency. A dead-layer that is too large will lead to charge loss as X-ray interact within the dead region causing a fall in charge cloud size and X-ray peaks that occur at incorrect energies. Errors in X-ray peak position will cause further degradation of the spectral resolution.

Radiation damage will have an effect on the end of life performance of the detectors used in an experiment; however, experiments have been performed that show the radiation damage effects in an EM-CCD are analogous to those in a CCD. The experiments suggest that conventional and EM-CCDs have the same radiation damage performance[21].

Finally, a decision is required as to whether spectral or spatial resolution should be optimised for the instrument. If interaction position on the CCD is the limiting factor on the instrument resolution, then split events can be maximised through the use of small pixels and large field-free regions. The centroiding of these split events would then give spatial resolution to sub-pixel accuracy, but at a cost to the spectral resolution. To maximise the spectral resolution the events should be confined entirely within a single pixel. Isolated events can be optimised using fully depleted, high resistivity silicon and large pixels, either through changing the device architecture or with “on-chip” binning.

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