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Electron-multiplying CCDs for future soft X-ray spectrometers

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ABSTRACT: CCDs have been used in several high resolution soft X-ray spectrometers for both space and terrestrial applications such as the Reflection Grating Spectrometer on XMM-Newton and the Super Advanced X-ray Emission Spectrometer at the Paul Scherrer Institut in Switzerland. However, with their ability to use multiplication gain to amplify signal and suppress readout noise, EM-CCDs are being considered instead of CCDs for future soft X-ray spectrometers. When detecting low energy X-rays, EM-CCDs are able to increase the Signal-to-Noise ratio of the device, making the X-rays much easier to detect. If the signal is also significantly split between neighbouring pixels, the increase in the size of the signal will make complete charge collection and techniques such as centroiding easier to accomplish. However, multiplication gain from an EM-CCD does cause a degradation of the energy resolution of the device and there are questions about how the high field region in an EM-CCD will behave over time in high radiation environments. This paper analyses the possible advantages and disadvantages of using EM-CCDs for high resolution soft X-ray spectroscopy and suggests in which situations using them would not only be possible, but also beneficial to the instrument.

KEYWORDS: Avalanche-induced secondary effects; Imaging spectroscopy; Spectrometers; X-ray detectors and telescopes

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1 Introduction

Electron-Multiplying CCDs (EM-CCDs) use on-chip gain multiplication to amplify the signal integrated in the charge packet before it is read out from the CCD [1]. The majority of noise is added to the signal through the readout process and, as the amplification of the signal occurs before the readout, the Signal-to-Noise in the image increases, causing the photons to be more easily detected. This gain multiplication does, however, cause a degradation in the energy resolution of the device which could affect high resolution soft X-ray spectrometer instruments using this energy resolution for order separation [2]. EM-CCDs achieve this gain on the signal through impact ionisation in a region of high electric field. This leads to concerns regarding the long-term stability of the gain register as ageing and radiation damage could cause severe degradation in the devices performance. This paper analyses the advantages and disadvantages of using EM-CCDs for high resolution soft X-ray spectroscopy with energy range 0.2 keV to 2.5 keV and addresses the concerns of EM-CCD operation in high radiation environments.
1.1 Current and future soft X-ray spectrometers

Several spectrometers are currently used in space and for terrestrial applications. In order to justify the manufacture of next generation experiments, their figure of merit can be a useful point for comparison. This is a measure of an instrument’s resolution and effective area. In order to broaden scientific understanding of the X-ray Universe, new telescopes need to have a higher figure of merit than previous missions. While Chandra has a higher resolution than XMM-Newton, they are both shown to have the same figure of merit (as seen in figure 1), whereas WHIMEx has a potential order of magnitude increase and the Reflection Grating Spectrometer on IXO has a potential two orders of magnitude increase in figure of merit, increasing the opportunity for the discovery of new science under extreme conditions [3]. Current and future space based X-ray spectrometer missions are discussed below, along with a terrestrial spectrometer.

1.1.1 The Reflection Grating Spectrometer, XMM-Newton

The Reflection Grating Spectrometer (RGS) on board XMM-Newton is a high resolution soft X-ray spectrometer \(E/\delta E > 300\) that operates between 0.35 keV to 2.5 keV [4]. The instrument consists of two On-Plane Gratings that disperse the incident X-rays over the two separate back-illuminated CCD arrays. Half of the X-rays collected by the telescope are diverted by the grating

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Figure 1. Spectral resolution at the OVII absorption line is shown verses effective collecting area for the past, present and potential future X-ray observatories. The diagonal lines are at constant figure of merit [3].
modules onto the CCDs and the other half go towards the main focus of the telescope. The RGS has been operating in a highly eccentric orbit (114000 km apogee, 7000 km perigee) since its launch in 1999. In order to achieve the necessary resolution and effective area across the RGS energy range, several dispersed orders at different energies are collected on the CCD array and the intrinsic energy resolution of the CCDs is used to distinguish between them. XMM-Newton and one of the back-illuminated CCD camera arrays (made up of 9 CCDs) on the RGS are shown in figure 2.

1.1.2 The Low and High Energy Transmission Gratings, Chandra

Chandra contains two transmission gratings that can be moved in and out of the telescope beam. The Low Energy Transmission Grating (LETG) operates between the 0.08 keV to 2 keV energy range and the High Energy Transmission Grating (HETG) operates between 0.4 keV to 8 keV. These instruments have a resolution ($E/\delta E$) of 300 at energies below 3 keV. Chandra has also been operating in a highly eccentric orbit (133000 apogee, 16000 km perigee) since 1999. Chandra has a moveable Advanced CCD Imaging Spectrometer (ACIS) that is designed to accommodate the different transmission gratings, but thanks to this design, the Chandra CCD array has been able to avoid much of the expected radiation damage by moving the CCDs out of the main focus of the telescope as it travels through the Earth’s radiation belts [5]. The Chandra telescope and the ACIS are shown in figure 3.

1.1.3 WHIMEx

WHIMEx is a bespoke X-ray spectrometer mission that is being proposed as a NASA explorer mission. It is designed to identify the Warm-Hot Intergalactic Medium (WHIM) that is thought to be the location of the missing baryonic matter in the Universe; however, in order to see this matter in absorption features, an order of magnitude figure of merit increase is needed from current X-ray missions. The instrument consists of a series of Off-Plane Gratings that disperse the X-rays in a conical fashion over the CCD camera array. The instrument is designed to have a resolution ($E/\delta E$) of $\sim$4000 over the 0.2 keV to 2 keV energy range. WHIMEx is designed to be able to produce much of the science that the Off-Plane X-ray Grating Spectrometer on IXO was designed...
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Figure 3. An artist impression of Chandra (left) and a photo of the ACIS (right) (Images from NASA).

Figure 4. The planned structure of WHIMEx (left) and the expected dispersion of the X-rays across the CCD camera array (right) [3].

to achieve [6], but has a figure of merit an order of magnitude lower (figure 1). It will be put into a 540 km Low-Earth Orbit with a 70° inclination and have a possible 5 year lifetime (3 years plus 2 year extension). Like the RGS, WHIMEx also uses the energy resolution of the CCDs to distinguish between different energy and order X-ray photons. The planned structure of WHIMEx and the dispersion expected across the CCD camera array is shown in figure 4.

1.1.4 The Off-Plane X-ray Grating Spectrometer, IXO

The Off-Plane X-ray Grating Spectrometer (OP-XGS) on the International X-ray Observatory (IXO) is a high resolution X-ray spectrometer (E/δE ∼3000) that was proposed to be part of a joint collaboration mission between NASA, ESA and JAXA. With its unprecedented size, IXO would have a large enough optic for the OP-XGS to achieve an effective area of greater than 1000 cm$^2$ over the 0.3 keV to 1 keV energy range. This large effective area and high resolution give the OP-XGS a figure of merit that is two orders of magnitude higher than any other mission currently in operation (figure 1). An artist impression of IXO and a CAD model of the CCD camera array are shown in figure 5.

The high resolution of this instrument can only be achieved by using several grating orders across the energy range and as a result the intrinsic energy resolution of the CCDs have to be used
Figure 5. An artist impression of IXO (left) and a CAD model of the CCD camera array (right) [8].

Figure 6. Position of X-ray photons of varying energy and order in relation to the distance the photons are from the zero order position for the OP-XGS. This shows that different energies at different orders overlap on the CCD array, making the energy resolution of the CCDs important in resolving out individual energies of photons [2]. For order separation [7] as is also the case on the RGS and WHIMEx. Figure 6 shows how different energies at different orders will overlap at the same position on the CCD array and so, in the OP-XGS instrument design case, the CCDs will have to be able to separate photons with energies that are 200 eV apart (600 eV photons in the 3rd order will fall at 180 mm from the zero order, as will 400 eV photons in the 2nd order). This puts a constraint on the energy resolution of the CCDs.
1.1.5 The Super Advanced X-ray Emission Spectrometer, PSI

The Paul Scherrer Institut (PSI) is a facility based just outside Zurich in Switzerland. It contains the Swiss Light Source (SLS), a high energy (2.4 GeV) synchrotron. One of the experiments at the SLS is the Super Advanced X-ray Emission Spectrometer (SAXES) that uses Resonant Inelastic X-ray Scattering (RIXS) to analyse samples [9]. This is a photon-in, photon-out process that uses the drop in X-ray energy to determine the samples characteristics. X-rays within the range of 400 eV to 1600 eV are incident on a sample, the X-rays are absorbed and then the sample fluoresces. The produced X-rays are dispersed by a grating across the face of a CCD and their spatial position across the CCD is used to determine the energy of the photons. In order to maximise the efficiency of this process, the highest possible spatial resolution is required and so techniques such as centroiding can be useful. The SLS facility at PSI is shown in figure 7 along with the SAXES instrument.

2 Electron-Multiplying CCDs (EM-CCDs)

EM-CCDs take a conventional CCD and add a multiplication register to the serial register before the output node. This can be seen in figure 8.

Accelerating the electrons in the charge packet through a large potential difference (40 V to 50 V) causes the number of electrons in the charge packet to be increased through “impact ionisation” [11]. The accelerated electrons have a probability, $g$, of impacting with an electron in the silicon lattice per gain element causing the electron to be excited to the conduction band. This acceleration occurs in each element of the multiplication register which is of the order 500 elements long, $N$. This allows a large amount of gain, $G$, can be added to the signal. This gain is described by the following equation:

$$G = (1 + g)^N$$  \hspace{1cm} (2.1)

Increasing the number of electrons in the charge packet relates to an amplification of the signal read out from the device. The readout noise stays the same regardless of the gain on the signal and so the effect of the readout noise is suppressed. This creates a number of advantages for using EM-CCDs. The noise suppression increases the detectability of signal integrated on the device (especially useful for small signal levels), readout speed can be increased as the increase in noise associated with faster readout is minimised and the noise suppression generates noise
immunity in the device (especially from Electro-Magnetic Interference (EMI)). EM-CCDs do have a disadvantage, however, as the gain multiplication process adds another component of noise to the signal which causes a degradation of the energy resolution [12]. The remainder of this paper will look in more detail at these advantages and disadvantages and help to identify whether EM-CCDs are suitable detectors for soft X-ray spectrometers. For simplicity and as is normal for X-ray spectroscopy with CCDs, the devices are assumed to be cold enough for dark current to be negligible (colder than -80°C).

3 Disadvantages of EM-CCDs for soft X-ray spectroscopy

While the increase in signal in the device has many benefits that are discussed later, the use of high voltage gain registers and the stochastic nature of gain multiplication can also lead to disadvantages with EM-CCDs. These problem are discussed below.

3.1 Energy resolution degradation

The stochastic nature of multiplication gain adds another component of noise to the detected signal. When using a CCD for the detection of X-rays, the Full-Width Half-Maximum (FWHM) of the detected signal is smaller than would be predicted using Poisson statistics. This is due to an effect described by Ugo Fano as the Fano Factor, \( f \) [13]. This factor describes the narrowing of the X-ray peak by 0.115 in silicon [14]. Through the use of gain multiplication, an additional noise has to be factored into the predicted FWHM of an X-ray peak. The extra component of noise has been described in optical applications as the Excess Noise Factor [10], but due to the difference in detection caused by the Fano Factor, it is described as the Modified Fano Factor in X-ray applications [12]. This factor can be used to predict the FWHM for a system with an EM-CCD operating at a variety of gains using Equation (2.1), where \( \sigma_{\text{readout}} \) is the readout noise in the device, \( \sigma_{\text{dark}} \) is the amount of dark current generated (negligible as the device is cold), \( G \) is the level of EM-CCD gain.
gain, $F_{\text{mod}}$ is the Modified Fano Factor, $E$ is the energy and $\omega$ is the energy required to generate an electron-hole pair in silicon [12, 15].

\[
FWHM = 2.355\omega \sqrt{\left(\frac{\sigma_{\text{readout}}}{G}\right)^2 + \sigma_{\text{dark}}^2 + F_{\text{mod}} \left(\frac{E}{\omega}\right)}
\]  

(3.1)

The amount of gain that is applied to the EM-CCD can have an effect on the amount of broadening that occurs in the X-ray peak. For a gain greater than 10x the Modified Fano Factor tends to $(1 + f) = 1.115$, but at lower gains the broadening is shown by figure 9 (left) and it becomes $f$ at a gain of 1x. The effect that this has on the detected signal can be seen in figure 9 (right) where the narrow peak is the Fano limited X-ray peak for the detection of Mn K$\alpha$ X-rays and the broader peak is what happens to the FWHM when multiplication gain of 10x is applied to the signal.

Figure 9 (right) clearly shows the degradation of energy resolution that occurs when multiplication gain is used and this can be problematic for X-ray spectrometers if the intrinsic energy resolution of the detector is needed to separate out different orders such is the case for instruments like the RGS, WHIMEx and the OP-XGS as discussed earlier. The Mn K$\beta$ peak can be seen to be lost in the K$\alpha$ peak for the case where a gain of 10x is applied, demonstrating the problem that the degradation of energy resolution can cause. If, in order to achieve the resolution and effective area goals of the instrument, several dispersed orders of X-rays are used, X-ray photons at different order and energy will be incident on the same part of the CCD. In order to distinguish between these photons, the intrinsic energy resolution of the CCD is used, but if the degradation of the energy resolution is sufficient enough this may no longer be possible. This means that understanding the degradation caused by using multiplication gain is important when it comes to spectrometer design.

3.2 Spurious charge

As EM-CCDs amplify all signal generated in the device, if the EM-CCD is warm enough and integration times are long enough that dark current becomes a significant proportion of the signal this dark current can be confused with photon interactions. The generation of dark signal in CCD
and EM-CCDs is well understood and reduces rapidly with temperature [1], but as the environment used for EM-CCDs is often a sparse photon environment, every generated electron is potentially significant. This means that cooling will have to be implemented on the device in order to suppress dark current generation as is the case with the CCDs on XMM-Newton [16] in order to remove the chance of dark current generated signal looking like a soft X-ray interaction.

This leads to a second problem with spurious charge generation. Parallel clock transitions, particularly those with fast edges, are known to generate spurious charge through the multiplication of holes in the column isolation region [1]. It occurs when the CCD is clocked into inversion as this allows holes to be trapped at the Si-SiO$_2$ boundary. When the clock is switched to a non-inverted state, the holes are accelerated from the Si-SiO$_2$ interface with sufficient energy to create electron-hole pairs through impact ionisation [17]. The effect is known as Clock-Induced-Charge (CIC). This is not a problem in a conventional CCD when detecting signal photons of a high enough energy, but with multiplication gain making all signal levels in the device increase, CIC can cause a problem in EM-CCDs as photon detection and CIC generated electrons can be confused. CIC is a form of impact ionisation and so it has a temperature dependence that follows the same trend as the EM-CCD gain multiplication process. This means that the CIC expected from a device gets higher as the temperature lowers [18]. The CIC experienced by a device can be lowered and so can be mitigated allowing for EM-CCDs to be used in photon starved environments. As CIC is generated by clocking into inversion, running the device in non-inverted mode will reduce the amount of charge generated. This may lead to an increase in dark current, but if the device is cold enough the increase will be negligible. CIC is also caused by fast clock transitions and so by running the clocks with longer rise and fall times, the spurious charge generated can be minimised [17]. This does limit the readout speed of the device, but as only the clock rise and fall times need to be lengthened the increase in readout time will be small. CIC has not been seen to be problematic in experiments with X-ray detection using EM-CCDs [12].

3.3 Temperature and gain stability

The amount of gain that is produced for a given voltage on an EM-CCD is highly temperature dependent and the amount of gain that occurs increases with decreasing temperature (figure 10). This is discussed in detail in [19]. CCDs used in X-ray applications are cooled in order to suppress dark current and maximise the Signal-to-Noise Ratio of the device. EM-CCDs are also run cold, but for the added reason, as discussed previously, that any dark current generation will be amplified by the multiplication register leading to the possibility of having signal confusion between photon interactions and dark signal generation. However, as EM-CCDs have a gain dependence on temperature it is vital that the temperature is held stable in order to not have fluctuating levels of gain. The level of temperature control required in order to maintain a constant gain level is of the order $\pm 1^\circ$, but this has been easily achieved on previous space missions [4, 16] and so should pose no problem to EM-CCD operation.

3.4 Power dissipation

The multiplication gain register on an EM-CCD has to be clocked at a higher voltage than you would expect on a conventional CCD. This leads to an increase in the power dissipation of the device and so extra cooling is needed to reach temperatures where dark current suppression is high
and extra power requirements have to be considered for the running of the device, especially in a space environment. The power dissipated by a clocking operation is approximated by:

$$P = C \times V^2 \times f$$  \hspace{1cm} (3.2)$$

where $P$ is the power dissipated, $C$ is the total capacitance of all the clock phases and they are being driven and a frequency, $f$, with amplitude $V$. If it is assumed that $C$ and $f$ are the same and the only difference between a conventional CCD and an EM-CCD is the clocking voltage then, with a normal CCD being serially clocked at 10 V and the gain register being clocked at 40 V, the power dissipation in an EM-CCD will be 16 times higher than in a conventional CCD. A typical CCD will produce 1 mW from the serial clocking that occurs to read out 50 rows from a device. An EM-CCD will also produce this power dissipation together with 16 times this amount for its multiplication register clocking. This amounts to an extra power dissipation though using an EM-CCD of 16 mW [21]. This will have to be taken into account in instrument design if an EM-CCD is going to be used, but as it is an easily predictable effect it should not be the reason that EM-CCDs are not considered for use on X-ray spectrometers, both on the ground and in space applications.

### 3.5 Gain ageing effect

EM-CCDs are known to age with use. The more that the devices are used, the higher the voltage needs to be in order to achieve the same level of gain. In order to mitigate this issue, e2v burn-in their devices before they are sold to customers in order to remove the period of highest degradation from the device. This feature of EM-CCDs has been studied. Unconditioned EM-CCDs were
run at a constant voltage and the level of gain that this voltage produced was measured over time. The initial rapid deterioration of the gain was seen, but over the duration of the testing after this initial drop (that occurs in the first few hours), the gain was only seen to fall by <0.2 V over 1300 hours of continuous operation [22]. Two EM-CCDs (CCD97s) were also run for 52 days to assess their avalanche gain stability as part of a suitability study for the Gaia RVS instrument. The experiment showed that, after the initial day of operation, the gain of the EM-CCDs were stable to within 10 % and both devices were able to reach the desired multiplication gain at the end of the test with an electrode voltage of less than 36 V. This suggests that, while gain deterioration does occur in the devices, the fall in gain is small and so can be easily modelled and corrected. The increase in voltage needed to correct the gain level on the device is also manageable and so gain degradation should not be a reason to overlook the use of EM-CCDs on high resolution soft X-ray spectrometers [23].

3.6 Radiation damage

EM-CCDs produce their multiplication gain by accelerating the electrons in the charge packet through a region of high electric field. There is some concern that radiation damage in this region of the device could lead to operational problems and possibly even device failure. For the Gaia RVS instrument, proton irradiation studies were performed up to a 10 MeV equivalent flux of $2 \times 10^{10}$ protons per cm$^2$. This is the expected flux that Gaia will receive during its lifetime at L2 [22]. The proton radiation study showed no degradation in the devices operable performance beyond that which would be expected in conventional CCDs [22]. In addition to this, 94 EM-CCDs were irradiated up to the Gaia expected lifetime flux and all devices remained functioning, there was no catastrophic device failure and dark current increase was as expected from a conventional CCD. This dark current increase did cause a reduction in the devices dynamic range, but, through cooling the dark current was suppressed and the dynamic range restored. Finally the amount of gain that would be expected for a given voltage was unaffected by the proton radiation and so the gain characteristics remained the same [24]. A gamma radiation [25] and heavy ion study have also been performed in order to see how the high electric field region reacts to the respective radiation damage. The gamma radiation study showed that the EM-CCD performed as would be expected from a conventional CCD and there was no catastrophic failure. The heavy ion testing was design to look for device failure through Single Event Gate Rupture, but this work has yet to be published. Radiation damage studies on EM-CCDs have found them to behave in the same manner as would be expected from a conventional CCD. They are no more prone to performance degradation or catastrophic failure than a normal CCD and so radiation damage effects consideration is not a reason to leave EM-CCDs off future space missions.

4 Advantages of EM-CCDs for soft X-ray spectroscopy

The multiplication of the signal on the device and the suppression of the noise that this creates has a number of advantages associated with X-ray detection.
4.1 Effective readout noise vs. readout speed

In order to minimise the readout noise in a system the CCD can be read out slowly. This limits the effect of thermal noise on the output signal as Correlated-Double Sampling (CDS) can be used to average out the fluctuations, minimising the overall readout noise. As the device is read faster, the CDS is less effective at reducing thermal noise, allowing its effect to increase and so the noise of the system also increases. This can be seen in the top line of figure 11.

Through the use of multiplication gain, this increase in readout noise can be suppressed as shown in figure 11. A gain of 2x and 10x applied to the signal produces a reduction of the noise at a given frequency. As the EM-CCD can be read out faster without the effective increase in readout noise affecting the signal, the device can be operated warmer for the same level of dark current per frame and sources with much higher flux rates can be observed without saturating the image because of the higher frame rate and throughput.

4.2 Improvements in X-ray detectability

Low energy X-rays generate relatively few electrons in the interaction in silicon (300 eV photons generate \( \sim 82 \) electrons) and so the events can be hard to detect above the noise floor of the image. This is especially true of events that are split across several pixels as even fewer electrons are available in each pixel to show the event above the noise. An EM-CCD would be able to amplify this signal before it is read out improving the detector sensitivity, allowing complete charge collection and making split events easier to identify. Figure 12 shows the effect of applying a gain of 7x to 1 keV and 0.3 keV X-ray photons. The increase in signal detection is especially clear in
the 0.3 keV case with the X-ray events becoming much more obvious above the noise even with a relatively low level of gain.

The increase in signal makes the split events more obvious and so can help with centroiding. Through looking at these split events it is possible to identify the position that the initial X-ray interaction took place with sub-pixel accuracy using method like centre of mass calculations for the X-ray charge in the pixels. If the spectrometer determines the energy of the incident photon through knowledge of the interaction position, this can improve the spatial resolution of the detector and so maximise the overall resolution of the instrument [26]. This increase in signal due to multiplication gain would be beneficial to experiments such as SAXES at PSI as the increase in potential centroiding will lead to a higher resolution of their instrument.

4.3 Increased noise immunity

Electro-Magnetic Interference (EMI) is caused by the electronics that surround the CCD. This EMI can setup patterns across the CCD that have an adverse effect on the noise. A pattern of this type can be clearly seen in figure 13, which is an example of the readout see from the RGS on XMM-Newton. Through multiplication gain the effect of this noise can be minimised.

An EM-CCD would have enabled the signal on the RGS camera to be amplified, suppressing the effect of the EMI and making the instrument less susceptible to fluctuations in the noise floor.

5 Conclusion

EM-CCDs have many benefits for soft X-ray spectrometers due to the amplification of the signal and hence the noise suppression that they can achieve. The noise suppression removes problems associated with EMI and readout speed as the signal detected in the device is amplified above the noise floor. The signal amplification also makes smaller signal levels more easily detectable in the device. This makes complete charge collection easier and split events become more obvious, helping with centroiding and hence makes sub-pixels spatial resolution possible. Experiments such
Figure 13. RGS spectra shown with an EMI pattern visible across the CCDs.

as SAXES at PSI will greatly benefit from such advancement as the increase in spatial resolution created will increase the overall resolution of the instrument. This makes EM-CCDs the ideal detector for this type of application.

If a future high resolution X-ray spectrometer requires the intrinsic energy resolution of the EM-CCD to resolve out different orders, as EM gain affects this energy resolution, their use may not be suitable.

While the use of multiplication gain causes the energy resolution of a device to degrade, it is a well understood and predictable effect that can be taken into account in instrument design and so should not be prohibitive in the use of EM-CCDs for soft X-ray spectrometers. It has also been shown that concerns about EM-CCD performance in high radiation environments is unfounded as there is no appreciable difference between the degradation of operation between conventional and EM-CCDs. Issues concerning spurious charge can be mitigated through cooling and well timed clocking operations and this cooling can be held steady enough to maintain a constant level of gain. There are issues regarding the ageing of the multiplication register, but after rapid initial decline this effect is small and manageable. EM-CCDs, due to their high clocking voltage, do have a higher power dissipation than their conventional counter-parts, but this is easily predicted and so can be catered for on soft X-ray spectrometers. With careful instrument design, EM-CCDs can be used for future soft X-ray spectrometers, making the advantages associated with noise suppression through signal amplification available.

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