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Considerations about future hard x-ray area detectors

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X-ray sources continue to advance in both intensity and temporal domains, thereby opening new ways to analyze the structure and properties of matter, provided that the resultant x-ray images can be efficiently and quantitatively recorded. In this perspective we focus on specific limitations of pixel area x-ray detectors. Although pixel area x-ray detectors have also advanced in recent years, many experiments are still detector limited. Specifically, there is need for detectors that can acquire successive images at GHz rates; detectors that can accurately measure both single photon and millions of photons per pixel in the same image at frame rates of hundreds of kHz; and detectors that efficiently capture images of very hard x-rays (20 keV to several hundred keV). The data volumes and data rates of state-of-the-art detection exceeds most practical data storage options and readout bandwidths, thereby necessitating on-line processing of data prior to, or *in lieu* of full frame readouts.

KEYWORDS

wide dynamic range, online detector processing, synchrotron radiation, x-ray burst rate detector, x-ray pixel array detectors

1 Introduction

X-ray analysis of matter has advanced greatly with the advent of brighter and more intense synchrotron radiation (SR) sources. This has enabled the development and application of techniques that were practically unfeasible only a decade or two ago. Examples include the real-time monitoring of microstructural details during materials synthesis (e.g., 3-D printing, thin film processing), nanometer-level ptychography of complex non-periodic objects (e.g., bone, integrated circuits, alloys), rapid optimization of the composition of multi-component thin-film catalysts, etc. In all these cases, improved x-ray sources enable experiments by providing the required numbers of x-rays arriving at the specimen with requisite time-structure, divergence, photon energies, and focal spot size.

However, getting x-rays to the sample is only part of the challenge: One must also efficiently detect the x-rays emanating from the specimen. X-ray detection technology has historically lagged source development and continues to constrain practical performance of many experiments.

The purpose of this perspective is to draw attention to several detector limitations presently constraining specimen analysis. It is impossible in a short Perspective to cover all types of experiments done at SR sources, or on all types of detectors. The focus here will be on “direct” (see below) detectors for very hard (>20 keV) x-ray diffraction experiments at both storage ring and XFEL applications. The focus will also be limited to integrating pixel array area detectors because photon-counting detectors cannot handle many x-rays/pixel/x-ray pulse often encountered at modern storage rings and XFELs [1].

2 Detector limitations: where are the needs?

2.1 Burst rate imaging

Much of the Universe consists of "warm, dense matter" in stars and planets where the densities are greater than Earth surface solids and the constituent atoms or ions have eV-scale thermal energies. Pulsed laser heating can produce transient warm, dense matter in the lab but it quickly explodes; hence, a need to capture x-ray images very quickly. SR sources can deliver sufficiently intense successive x-ray pulses at very fast rates, thereby enabling study of warm, dense matter dynamics. This requires "burst-rate detectors" [1] to record successive diffraction patterns, or "frames" within the time envelope of the event, typically in the ps to μs range. Other experiments requiring burst-rate detection include analysis of shock waves and study of crack propagation and materials failure under sudden stress.

Burst-rate detectors may utilize either "direct" or "indirect" detection of the results of x-ray absorption in a "sensor screen". In the former, x-rays absorbed in a sensor screen, such as a sheet of appropriately biased semiconductor, produce electron-hole pairs. This yields an electrical current that is directly processed by in-pixel electronics. Indirect detectors use a sensor screen that produce other types of quanta, such as visible light from a scintillator that is then recorded by a camera. Attention in this short Perspective is confined to direct detection.

State-of-the-art burst-rate detectors frame at nearly 1 GHz [2–5], a rate that is too slow for processes occurring on ps time scales but adequate for slower processes. A primary limitation is the detector readout rate: Even at 10 MHz framing, a 1B/pixel full-frame readout of, say, 10^5 pixels implies an off-detector data rate of 10^{12} B/s; this is beyond current capabilities. In practice, a small number of frames (~10) often suffices; hence, state-of-the art burst-rate imagers store images in-pixel for later, much slower readout after the experiment is over. Going beyond 10 MHz framing will require new technology, e.g., faster in-pixel electronics and more intelligent readout schemes. In most high-frame rate situations the images consist of mostly null pixels. This is because even x-ray bursts delivered to a sample from an XFEL tend to top out at ~10^{12} x-rays, only a small fraction of which are scattered over the many pixels of the detector. In-pixel electronics that reject null events from readout ("sparsification") can greatly reduce the required detector readout rate, an approach typical of many high energy physics detectors.

2.2 Continuously framing, wide dynamic range imaging with single x-ray sensitivity

Another class of experiments requires very many frames in which the x-ray dose/pixel/frame may vary over 5 or more decades. Examples include high spatial resolution ptychography of extended objects (e.g., bone, integrated circuits, composites), dynamic SAXS, and simultaneous collection of Bragg and diffuse scatter from labile crystals. Often the weak parts of the image are photon starved, thereby necessitating single x-ray detection sensitivity, even as the low-Q diffraction receives many millions of x-rays/pixel/frame. Note that most such experiments rarely require measurement of the x-ray dose per pixel to better than a few tenths per cent accuracy. This is fortunate because detector calibration errors and x-ray Poisson noise would otherwise impose limitations. (Users are often surprised to discover that practically all area detectors on SR beamlines are not calibrated to better than 0.5% accuracy.)

Most fast, continuously framing cameras use a charge-to-voltage converting amplifier to integrate the charges resulting from x-ray absorption in the sensor screen. This amplifier operates between fixed voltage limits, V_{SAT}, of typically less than a few volts. All amplifiers have some front-end noise, σ_{IN}. Robust single x-ray detection requires that the signal, S, from a single x-ray be such that $S \approx 5\sigma_{IN}$. For a linear amplifier, the dynamic range, D_R is then < V_{SAT}/S x-rays; this is typically in the range of 10^2–10^4 x-rays. Larger values of D_R could be obtained with an amplifier with a nonlinear (e.g., logarithmic) response at the cost of complex calibration. A detector with a high-gain linear amplifier can have an extended dynamic range *via* implementation of electronics that remove fixed quantities of charge from the feedback integration capacitor as the signal accumulates. This dynamic integrator charge removal scheme is the basis for the Mixed-Mode Pixel Array Detector (MM-PAD) family [6–8]. Some examples of other detector efforts exploring high sensitivity, wide dynamic range realm include JUNGFRAU [9], AGIPD [10], CITIUS [11, 12], and CoRDIA [13].

2.3 High atomic weight (hi-Z) sensor screens

Sensors providing high quantum efficiencies for very hard X-rays (>20 keV) are critically important to extend effective photon science beyond the reach of existing silicon sensors. The development of silicon x-ray sensors leveraged processes originally developed for the microelectronics industry with modifications and customizations required for the full silicon-thickness usage. However, high-quality, hi-Z sensors have not had this luxury. The technical challenges of hi-Z weight sensors are in several elements of sensor production, e.g., synthesis of crystals of sufficient size and quality, fabrication of pixelated sensors with the required pitch, and the *ad hoc* processes for integration and bonding to multipixel ASICs. Hi-Z sensors must have not only good energy resolution, temporal stability, homogeneity, carrier mobility (μ) and lifetimes (τ), low lag and dark current but also equally important must be readily available. Recently, the medical imaging industry has turned its attention towards "direct" detection computed tomography (CT) systems (e.g., photon counting CT and SPECT-CT imaging), resulting in the availability of new hi-Z weight sensors.

One of the first hi-Z weight sensor material to be readily available commercially for photon science applications is Cadmium Telluride (CdTe) [14]. Currently, CdTe offers a compromise between performance and availability while simultaneously providing some degree of radiation protection to underlying electronics. CdTe is arguably the predominate hard x-ray sensor used for commercial high energy x-ray pixel array detectors. However, CdTe sensors are prone to the buildup of excessive space-charge at relatively modest flux available at storage rings and XFELs. Cadmium Zinc Telluride (CZT) has been extensively used for low-flux spectroscopic applications. Recently, so called 'high-flux-capable' grade CZT from Redlen [15] appears to hold great promise, but the availability for photon science applications has been challenging. This variant of CZT has been designed with more nearly equal μτ-product for both holes and

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electrons compared to its low flux equivalent [16]. The resulting material has shown stable performance at very high flux, even under conditions observed at XFELs [17]. Gallium arsenide (GaAs) sensors have also garnered attention for moderate hard x-ray energies. Unlike CdTe or CZT, GaAs lacks a troublesome absorption edge above 20 keV. A number of groups have examined the considerable promise of chromium-compensated gallium arsenide (GaAs:Cr), though obtaining material of sufficient and consistent quality, area and thickness has been an issue [18–20]. There are currently two sources providing GaAs:Cr for x-ray science detector applications [21, 22]. Besides availability, prominent problems with GaAs:Cr include lengthy charge collection times and nonlinearities [18, 23]. Finally, new classes of hi-Z materials such as perovskites (e.g., $CsPbBr_3$) are being studied for radiation detection [24, 25], but significant R&D will still be required.

The sensor materials discussed above are generally single crystal boules that are processed into thick (>0.5 mm) wafers. There is another class of sensor materials that are grown using thin film techniques (e.g., physical vapor deposition or molecular-beam epitaxy (MBE)) for moderate x-ray energies. Amorphous selenium (a-Se) sensor screens have been used by the medical imaging industry for static applications, such as mammography. Time-resolved, high-dynamic range imaging with a-Se sensors have been hindered by flux-dependent afterglow issues [26, 27], but there are applications in photon sciences requiring simultaneous high-energy and high-spatial resolution at low-flux levels [28]. CdTe [29] and GaAs [30] can also be grown using MBE deposition techniques; these materials show promise for ultra-fast applications, e.g., [31]. Solution-processed perovskite thin films are being studied [32].

Finally, the collection rate of quanta resulting from the absorption of x-rays is an important consideration for burst-mode imaging approaching GHz frame rates. In direct detection the thickness and carrier mobilities of the x-ray absorbing layer are key parameters for both detector quantum efficiency and temporal response. This is especially true for the hi-Z sensor screens required for very hard x-rays. Si sensor screens thick enough to efficiently absorb >20 keV x-rays require ~10s of ns to collect charge into the input node of the collection electronics [33, 34]. Hi-Z semiconductors with higher carrier mobilities than Si are known [35] but few of these are available in the quality or size needed for direct x-ray detection. This is yet another reason to continue to develop new hi-Z sensors.

2.4 Continuous on-line image analysis

The combination of increases in detector frame rates and pixel number, together with the evolution of multimodal and concurrent techniques, challenge existing capabilities in data acquisition, online fast feedback, and computing capacity. Currently, detectors and data reduction methods are not tightly integrated. In addition, the continued demand for faster detectors presents severe challenges of limited data bandwidth off the detector front-end and of the deluge of data that such new detectors will generate. The flood of data also limits the ability of scientists to extract actionable insights to steer experiments. It is estimated that the U.S. light sources will generate exabytes (EB) of data over the next decade, requiring tens to 1,000 PFLOPS of peak on-demand computing resources, and utilization of billions of core hours per year [36]. Data loads of TB/s at LCLS-II, 1.3 EB per year at SPring-8 and similar loads at the European XFEL [36, 37] can only be managed by the implementation of strategic data reductions as close as possible to the signal generation point, i.e., edge processing. Light sources around the world are developing strategies for data reduction at different stages of the data flow. Several tradeoffs should be considered when choosing how early data reduction can be implemented effectively. Reconfigurable and flexible implementations can occur directly after the first front-end readout functions or further downstream of the detector [38, 39]. However, they require significant bandwidth and massive parallelism for data streaming. On the other hand, specialized hardware solutions offer the opportunity to send out only selected data with optimal information content. Dedicated readout architectures can be designed to optimize data quality and implement pre-processing, e.g., reconstruction of partial signals shared between pixels to improve either position or energy resolution while reducing the number of pixels to be recorded [40]. They can be specific to a typology of scientific data and require advanced technologies to achieve suitable processing density while maintaining reasonable power consumption.

A concern when implementing any type of reduction technique is if important information is lost that might alter the result of an experiment. Lossless data compression is an efficient and popular option that can be achieved by zero suppression at the detector readout level or at successive intermediate steps and offline (e.g., frame summing, Hcompress). The former requires dedicated readout architectures that work only for some categories of experiments. In some cases, selections of relevant regions of interest are also possible *via* relatively simple hardware and software options; this allows a focus on key information at the timescale important for the phenomena being investigated. Suppressing redundant information in the data stream may also be achieved with the acceptance of some losses. Lossy compression is very much experiment-specific and requires user involvement to evaluate quality and value of the different implementations.

The use of artificial intelligence and/or machine learning inspired data handling for on-line images analysis is becoming very popular. Pattern identification and recognition can be a powerful method to improve performance and efficiency. It allows identification of the class of problems and associated solutions, as has been studied for light source applications [41]. For example, online autonomous Bragg peak finders and analysis are much sought after and new tools utilizing deep neural networks are now becoming available [42, 43].

As mentioned earlier, on-detector electronics to reduce data flow is very promising and is being explored in various fields [44]. At the other end of the implementation space, predictive approaches are also becoming very popular and can help optimize data flows (e.g., compression ratio and speed), but typically require careful validation [45, 46].

3 Conclusion

Advances in pixel area x-ray detection will be needed to exploit capabilities provided by the rapid advance of x-ray sources. New technologies, materials, and concepts provide great opportunities for advancement in the next decade. In this Perspective we noted some of the challenges (i.e., frame rate, dynamic rate, high-energy sensors and on-line data analysis) and point to the current state-of-the-art. There is much yet to be done.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

SG: Conceptualization, Writing–original draft, Writing–review and editing. GC: Writing–original draft, Writing–review and editing. AM: Writing–original draft, Writing–review and editing.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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