White paper

The perfect match of 24 keV MetalJet and CdTe HPC detectors

Enabling high-energy synchrotron applications in the lab.

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1. Introduction

Over the past two decades, rapid advancements in hybrid photon counting (HPC) detectors[1], and extreme-brightness Gallium MetalJet X-ray source technology have significantly expanded and improved the use of various X-ray methods, including single-crystal and powder X-ray diffraction (SC-XRD, PXRD)[2], small-angle X-ray scattering (SAXS)[3], computed tomography (CT) [4], and others. These developments have also enabled highly challenging applications that were previously only feasible at synchrotrons. For instance, small and weakly diffracting crystals of proteins, metal-organic frameworks, and pharmaceutical compounds can now be studied using SC-XRD in a home laboratory setting, offering unprecedented convenience and accessibility.

Efficient data collection demands high quantum efficiency detectors. Silicon sensor-based HPC detectors have very high quantum efficiency, of up to 98% at lower energies (below 12 keV). In such cases, a Gallium MetalJet source emitting 9 keV characteristic radiation[5], combined with an HPC detector featuring a Silicon sensor, provides an optimal setup by delivering high flux and high quantum efficiency at the relevant energy range. For higher energies, provided by X-ray sources such as the Indium MetalJet, a different sensor material is needed. CdTe has been utilized in detectors thanks to its high quantum efficiency for X-ray energies up to 100 keV[6,7].

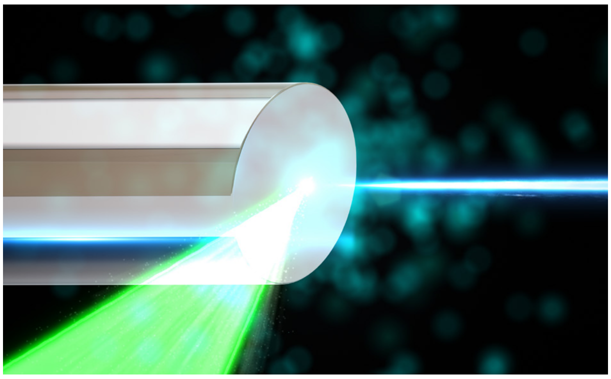
The combination of the Indium MetalJet sources with HPC technology with CdTe sensors provides a unique opportunity for novel high-energy experiments that were previously impossible to conduct in laboratory environments. Typical examples of applications that require harder X-ray radiation include, transmission-XRD, -SAXS and -WAXS, where the higher energy photons improve penetration through thicker and denser samples. High-pressure XRD is another area where increased photon energy allow for more efficient penetration of the diamond anvil cell (DAC), which is crucial for investigating materials under extreme conditions[8]. A key limitation in DAC experiments is the restricted access to diffraction reflections due to the gasket and sample holder geometry. Higher-energy X-rays with shorter wavelengths compress the reciprocal space, granting access to additional reflections and improving data completeness. Additionally, for high-resolution studies such as charge density measurements, using higher-energy radiation enhances resolution and allow for more precise electron density calculations.

While these high-energy X-ray applications are traditionally conducted at synchrotron facilities, there is increasing interest in bringing them to the laboratory setting to reduce dependence on large-scale research infrastructures and accelerate innovation. However, implementing high-energy X-ray techniques in a home lab presents significant challenges. First, conventional X-ray sources struggle to generate sufficient flux at high energies due to the limitations in photon yield, especially at the relatively low acceleration voltages (50–60 kV) typical of standard laboratory sources. Second, at higher energies, the efficiency of X-ray optics decreases as both reflectivity and collection angles are reduced, leading to significant photon losses before reaching the sample. Finally, on the detector side, traditional sensor materials exhibit low absorption efficiency for high-energy X-rays, as these photons tend to pass through the sensor with minimal interaction.

The purpose of this white paper is to explore the synergy between Excillum's pioneering high-energy Indium MetalJet X-ray sources and DECTRIS's advanced CdTe HPC detectors. By combining these two state-of-the-art technologies, new possibilities in high-energy diffraction and scattering applications can be unlocked, bridging the gap between synchrotron-based research and laboratory-scale experimentation.

2. The liquid-metal-jet concept

The Excillum MetalJet X-ray tubes are similar to conventional microfocus tubes where the solid-metal anode is replaced by a liquid-metal-jet[9]. This type of anode is continuously regenerated and is already in the molten stage. Thereby, the classical power limit of an X-ray source, when the anode is permanently damaged (melted) by the electron beam, is no longer a problem. In this way the metal-jet technology supports extremely high electron-beam power densities. In comparison, an overview of different X-ray source technologies and related electron beam power density is provided in the table below. Corresponding brightness and radiant flux from each source are, besides the e-beam power density, dependent on several other factors including target/anode material, acceleration voltage, take-off angle and line focus.



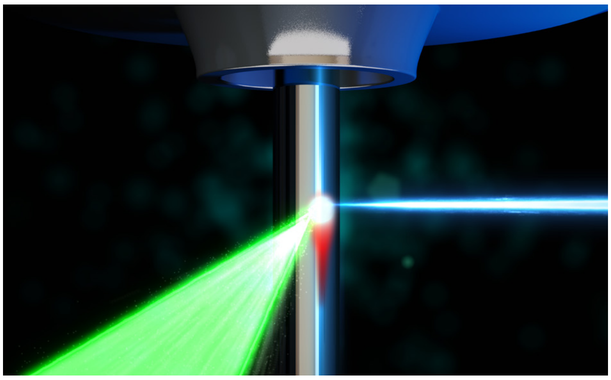


Figure 1:
Regular anode (left) – E-beam hits a solid target, which limits the amount of electron beam power that can be applied to prevent damage. Liquid metal-jet anode (right) – A fast-moving MetalJet target constantly supplies new material, efficiently transporting away released energy and enabling significantly higher power loads.

Source	Typical Max Power	Typical Electron Beam Size	Typical X-ray spot size*	Electron beam power density **
Standard sealed tube - 60 kV	3000 W	0.5 X 10 mm²	500 µm	~0.6 kW/mm²
RAG (rotating anode generator) - 60 kV	18 000 W	10 X 0.5 mm²	1000 µm	~3.6 kW/mm²
Sealed microfocus source - 50 kV	30 W	30 X 120 µm²	30 µm	~8 kW/mm²
µRAG (microfocus rotating anode) - 60 kV	1200 W	70 X 700 µm²	70 µm	~25 kW/mm²
µRAG (microfocus rotating anode) - 60 kV	3000 W	70 X 700 µm²	70 µm	~60 kW/mm²
MetalJet - 70 kV	250 W	20 X 80 µm²	20 µm	~150 kW/mm²
MetalJet - 70 kV	250 W	10 X 80 µm²	10 µm	~300 kW/mm²
MetalJet - 160 kV	1600 W	20 X 120 µm²	30 µm	~650 kW/mm²

** This is the apparent X-ray spot size as seen from the X-ray source window, it is commonly created by an electron beam line focus impact on a target at a take-off angle, creating an approximately round apparent spot. Note that apparent spot size also depends on the acceleration voltage of the source.*

*** Power density is power divided by the electron beam size.*

In order to reach different X-ray emission lines, different metal alloys are used. MetalJet sources feature metal alloys that are molten at more or less room temperature. Still, several alloys have emission characteristics similar to regular solid anodes. For high-energy applications an indium (In) rich alloy has a Kα emission of 24.2 keV (0.51 Å) which is higher than silver (Ag) Kα emission line at 22.1 keV (0.56 Å). Besides the extreme power density of the electron beam the Indium MetalJet also supports operation up to 160 keV that efficiently excites the Indium Kα line at 24 keV and can therefore generate very high 24 keV X-ray brightness. A spectra (flux vs energy) of Indium MetalJet at 160 keV compared with a silver anode is provided below. The In Kα emission line is significantly stronger than the silver line, and the In Kβ line is stronger as well.

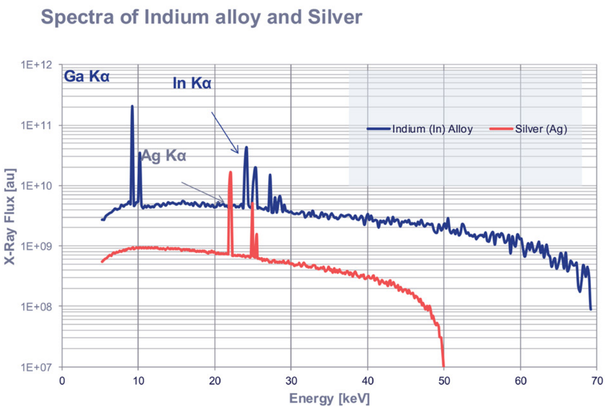


Figure 2: X-ray Spectra (flux vs photon energy) of a MetalJet source with Gallium, Indium and Tin target alloy illustrating access to several high energy characteristic lines. As comparison spectra for a solid silver anode source is shown.

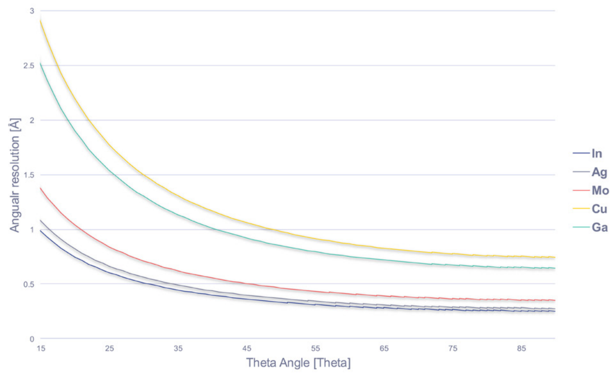


Illustration of attainable resolution for the most common anodes materials used for scattering and diffraction.
Indium gives the hardest X-ray, leading to the highest possible resolution.

As seen in the table above, the latest MetalJet platform has a total power of 1600 W emitted from a ~30 µm X-ray spot at 160 kV acceleration voltage. The combination of extreme power density paired with very high acceleration voltage enables extremely bright micro-focused 24 keV characteristic indium Kα X-ray beams. The illustration shows an example of a monochromatic 24 keV X-ray beam of approximately 12 µm FWHM. The beam was created using a MetalJet E1+ source in combination with an AXO Montel mirror.

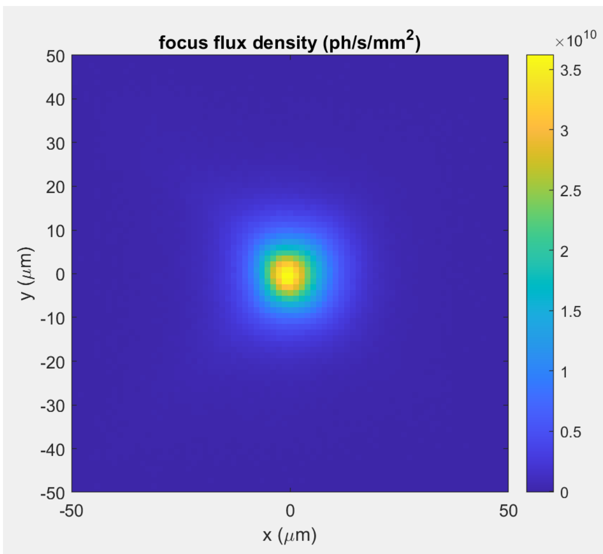


Figure 3: Pinhole camera image of 24 keV X-ray beam. Demonstrating X-ray beam focus size of around 12 µm FWHM

3. Hybrid Photon Counting detectors for high energies

The HPC detectors consist of a pixelated semiconductor sensor, with each pixel linked to a corresponding readout pixel on a readout chip beneath it. In this arrangement, every pixel is equipped with its own integrated circuits for single-photon counting, making it an independent point detector[1]. When photons are absorbed by the sensor, they generate a charge proportional to the energy of the photons. Because this charge, and therefore an electrical signal, is generated without any intermediate steps, this process is also referred to as direct detection of X-rays. A bias voltage across the sensor directs the charge to the input of the readout pixel, resulting in an electrical signal that is again proportional to the X-ray energy. If the signal exceeds an adjustable energy threshold, the readout pixel will count the photon by incrementing a digital counter by one, thereby achieving the earliest possible digitization in the detection process. In this way, photon-counting ASICs accomplish a high dynamic range, zero detector background, and fast frame rates.

Direct detection achieves exceptional spatial resolution, characterized by a sharp point-spread function that is just one pixel wide. It also enables high quantum efficiency (QE) close to the absorption efficiency of the sensor material. The most commonly used sensor material in HPC detectors is silicon. While silicon provides high QE for Cu radiation, the efficiency is increasingly reduced for the higher energies of Mo, Ag, and In radiation. HPC detectors equipped with CdTe sensors resolve this issue thanks to the larger absorption efficiency of their sensor material, resulting in superior QE for all radiation energies commonly used in diffraction and scattering experiments performed with laboratory sources.

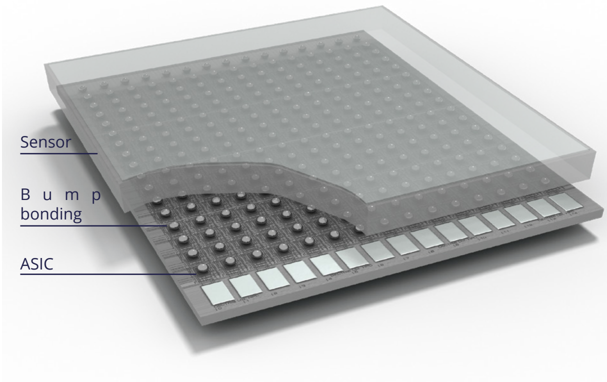


Figure 4: Schematic rendering of an HPC pixel detector

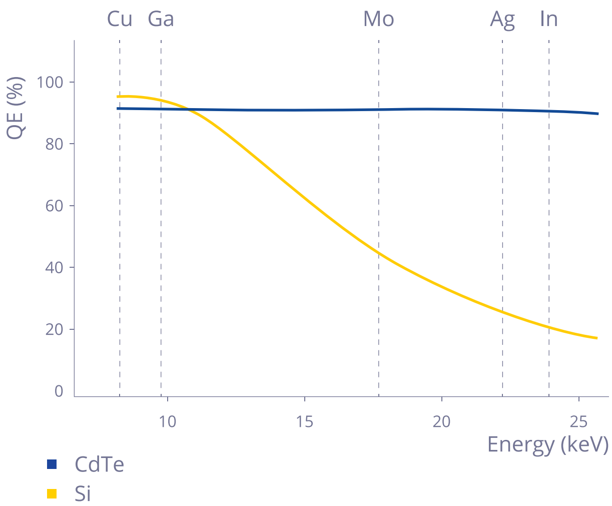
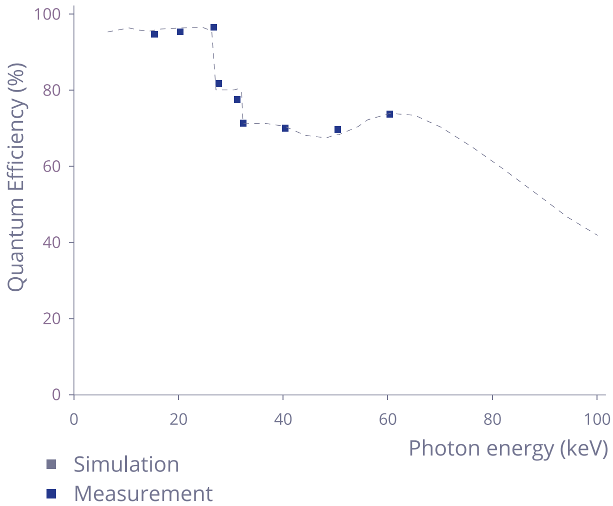


Figure 5: Quantum Efficiency of EIGER2 detectors with 750 µm thick CdTe (blue line) or 450 µm thick Si (grey line) sensors.



The Quantum Efficiency of CdTe sensor detectors for energies up to 100 keV.

4. Laboratory revolution on high energy experiments

As discussed above, the Indium MetalJet source is capable of providing a very bright 24 keV X-ray beam. This is particularly beneficial for diffraction and scattering experiments, where higher photon energies can penetrate denser materials or thicker samples, and provide improved angular resolution and signal-to-noise ratio for scattering profiles. To fully utilize this higher photon flux, HPC CdTe detectors are an ideal match, especially for their high QE at energies in this range. The CdTe sensors in DECTRIS detectors achieve QE values greater than 90%, between 8 and 25 keV (Figure 5), ensuring optimal detection efficiency, which is crucial for capturing weakly diffracted or scattered photons and allowing researchers to collect accurate data with fewer exposures or faster data collection times. As the characteristic K edges of Cd and Te are at 26.7 keV and 31.8 keV respectively, the Indium source is the perfect match as we are below them.

The high flux density of the Indium MetalJet source requires a detector capable of handling intense beams without saturating or losing photon information. DECTRIS EIGER2 and PILATUS4 detectors are built with high dynamic range, ensuring that both strong and weak signals are captured accurately because of the zero noise. The high count rate capability of these detectors, reaching up to 10^6 counts per second per pixel, makes them ideal for high-flux environments typical of diffraction and scattering experiments with MetalJet sources. This feature is particularly important in high-throughput diffraction or high-energy scattering, where the detector must capture data at high speeds and handle the intense diffraction peaks or scattering events produced by the focused, high-flux beam of the MetalJet source.

The Indium MetalJet sources generate highly focused X-ray beams, making them ideal for diffraction and scattering experiments that require small, micro-focused beam sizes. The small spot sizes of the Indium MetalJet source require detectors with fine spatial resolution to accurately map diffraction patterns or scattering intensities. The EIGER2 series detectors have 75x75 µm pixel size, which is critical for achieving optimal spatial resolution in diffraction patterns or scattering profiles. This small pixel size ensures that even small angular changes in scattered or diffracted beams are detected with precision. The one-pixel-wide point spread function which is enabled by the direct detection of DECTRIS detectors, further ensures minimal signal blurring between adjacent pixels, a critical feature when resolving fine diffraction spots or detailed scattering patterns.

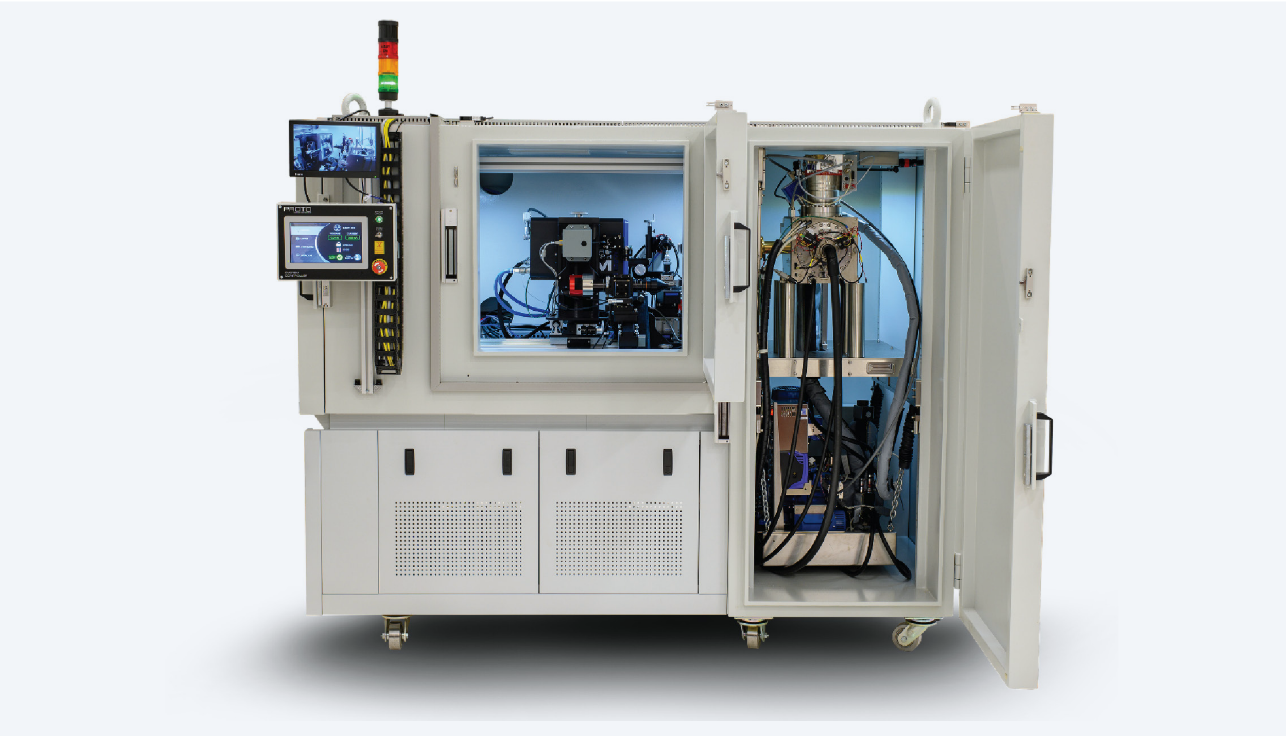


Figure 6: An example of a High Pressure X-ray instrument from PROTO combining an EIGER2 CdTe 4M detector with a In MetalJet source.

5. Conclusion

The synergy between Gallium MetalJet X-ray sources and HPC detectors in lab systems has for many years enabled a leap forward in a multitude of fields from chemistry, biology, material science and beyond. This combination offers researchers and professionals unprecedented insights and powerful tools to efficiently solve their challenges in the convenience of a home lab. The latest developments in MetalJet X-ray source with Indium alloy are now bringing a revolution in enabling in-house high energy X-ray beams. At the same time, due to their high quantum efficiency and high dynamic range, the Cadmium Telluride (CdTe) sensor EIGER2 or PILATUS4 series detectors are the optimal choice to fully exploit the high energy beam from an Indium MetalJet source. Therefore, the combination of the two systems is the perfect match for hard X-ray applications. These combined technology instruments are provided, for instance, by PROTO and can also be implemented by other lab instrument manufacturers.

6. References

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