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Report on the Photocathode Options for a UK X–ray Free–Electron Laser

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Summary

This report summarises the photocathode options for a UK X–ray Free-Electron Laser (UK XFEL). It draws on the reports of photocathode solutions and their measured performance from a number of laboratories around the world to deliver high brightness and/or high repetition rate electron beams. Initially the UK XFEL baseline design considered operation at a low electron bunch repetition rate (‘LRR’: 1 – 100 kHz in a normal–conducting NcRF gun), or at a high repetition rate (‘HRR’: 1 MHz or more in a normal–conducting [NCRF] or a super–conducting [SRF] gun). The project now focuses on the delivery of a HRR machine with up to 300 pC electron bunches at MHz bunch rate (0.30 mA beam current, or more), with slice emittance of 0.3 μm at 8 GeV beam energy for a 250 pC bunch charge. Such a beam can be used to generate coherent 20 keV X–ray photons which will meet the experimental requirements of a substantial majority of the potential user community. The final machine design may incorporate an energy recovery linac (ERL), and the corresponding need for a cryogenic plant supports the possible development of an SRF injector to deliver the beam. There are several photocathode technologies which have the potential to meet these beam requirements, most notably the semiconductor Cs_2Te and bare metals such as Cu, Mg or Mo under illumination at UV wavelengths (typically 266 nm), or bi–alkali semiconductors such as CsKSb, NaKSb or CsSb under illumination at visible ‘green’ wavelengths (532 nm). While the green photocathodes are generally more attractive due to their high quantum efficiency and the corresponding simplification in the required drive laser technology, there are potential issues with the operational lifetime of these technologies in a high–current injector. The Cs_2Te and plain metals are demonstrably more robust, but carry the penalty of a more complex and expensive drive laser system.

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1 Electron Beam Brightness

The UK X–ray Free–Electron Laser (XFEL) injector will require high–brightness electron bunches at a high repetition rate. The injector will be based on an RF photoinjector designed to deliver a pulse train at 1 MHz or more with electron bunch of up to 300 pC. The drive laser pulse length will be adjusted to extract this bunch charge at the space–charge–limited threshold.

The fundamental factors limiting beam brightness are the electric field at the photocathode surface and the intrinsic emittance of the photocathode material [1]. By extension, photoinjectors containing low intrinsic emittance photocathodes deliver the highest possible levels of electron beam brightness.

The concept of beam brightness was introduced by Ruska [2] in relation to beam quality within electron microscopes. This was based on a 5D framework involving peak current (I) and emittance (beam size and divergence) (ε_n) with $B_{5D} = 2I/\varepsilon_n^2$. However, B_{5D} is not invariant within the current linear accelerator technology, so this duly evolved into a framework based on the 6D phase space (B_{6D}) which is preserved in a Hamiltonian transport system through the Liouville theorem [3].

The Shamuilov space charge model for photoinjectors [4] takes the generalised 2D Child–Langmuir model developed by Lau [5] and derives a more accurate generalised model for an emission area of arbitrary radius which recognises the inter–slice forces present during photoemission. Filippetto previously extended the Lau model for a photoinjector, recognising that the <longitudinal> length (D) of the electron bunch extracted from a photocathode is generally much greater than the <transverse> radius (R) such that $D >> R$ [6], however this causes a discrepancy as the predicted current density for the 2D Child Langmuir model is 25 % larger than that for the 1D model. The Shamuilov model predicts that the maximum current density is extracted from an annular or elliptical beam footprint on the cathode surface as the transverse space charge force diminishes more quickly in these beam profiles than in a Gaussian or cylindrical pattern.

While Shamuilov has shown that the aspect ratio of the bunch emission footprint on the photocathode surface limits the maximum 2D current that can be extracted, the peak brightness limit is directly related to the surface electric field, so justifying the technological push towards achieving and sustaining high electric field gradients on the photocathode surface. The 3 generic classes of photoinjector gun technology are:

1. Direct current static voltage (DC)
2. Normal-conducting radio frequency (NCRF)
3. Super-conducting radio frequency (SRF)

All of these gun classes are capable of maintaining cathode surface fields of around 10 MV/m at a high repetition rate of 1 MHz or more. The NCRF and SRF classes are capable of sustaining substantially higher surface field levels than this, their upper limit being dictated by their RF frequency [reference ??]. However, only the NCRF and SRF gun classes can achieve the levels of beam brightness required by a UK XFEL.

Many factors affect the energy spread of the photoemitted electrons, and the delivery of optimal performance and beam quality in an electron accelerator necessitates the minimisation of this energy spread. The mean transverse energy (MTE) is a readily measurable photocathode performance metric [7, 8], and MTE couples directly into intrinsic photocathode emittance (ε_i) which convolutes in quadrature with the beam transport emittance (ε_t) and so impacts B_{6D} and the ultimate achievable minimum electron beam emittance:

$$\varepsilon^2 \approx \varepsilon_t^2 + \varepsilon_i^2 = \varepsilon_t^2 + \sigma \cdot \frac{\mathrm{MTE}}{m_e c^2} \tag{1}$$

where σ is the laser spot size on the photocathode surface and m_e and c have their usual meaning. The precise illumination wavelength (λ) and the photocathode temperature (T) impact on the transverse energy spread present in the photoemitted electron distribution, and therefore on the MTE. In this way, electron source MTE and hence emittance can be reduced/minimised through adjustment of the illumination wavelength to shift the operating point closer to the photocathode emission threshold [9]. The minimum MTE achievable ($\mathrm{MTE}_{\mathrm{min}}$) is dependent on the photocathode temperature and is achievable only at the absolute photoemission threshold where the quantum efficiency (QE [1]) is vanishingly small. This energy is given by:

$$\mathrm{MTE}_{\mathrm{min}} = k_B T \quad [\mathrm{eV}] \tag{2}$$

where k_B is the Boltzmann constant. In order to ensure a usable level of QE and an acceptable level of MTE, we will aim to illuminate the photocathode at a wavelength such that the photon energy is approximately 1 eV more than the surface work function (ϕ). This excess energy translates into the photocathode MTE according to the relationship developed by Dowell and Schmerge [10], then extended by Vecchione to recognise non–zero temperature of the Fermi–Dirac electron distribution [11], and more recently generalised for photoemission from disordered surfaces by Saha [12]:

$$\mathrm{MTE} = \frac{e}{3} \cdot \left(\frac{hc}{\lambda} - \phi \right) \quad [\mathrm{eV}] \tag{3}$$

While the aspiration to illuminate the photocathode at a photon energy which is ~ 1 eV above the work function is somewhat arbitrary, the actual illumination wavelength chosen must be a standard commercial laser wavelength in order to access the required levels of optical power necessary to extract a bunch charge in the region of 300 pC at MHz repetinio rates.

Metal photocathodes illuminated by a femtosecond or picosecond UV laser can act as ultra–fast electron sources for particle accelerator applications. Generally polycrystalline metal surfaces are

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[1] QE is defined as the simple ratio between the number of emitted electrons and the number of incident photons.

used as photocathode electron sources. Such photocathodes are capable of providing very short electron bunches, albeit with a low level of QE. Whilst their efficiency is poor when compared to other photocathode classes such as positive or negative electron affinity semiconductors, they are typically quite robust and perform as reliable and consistent electron sources for a substantial period of time.

2 UK XFEL Specifications

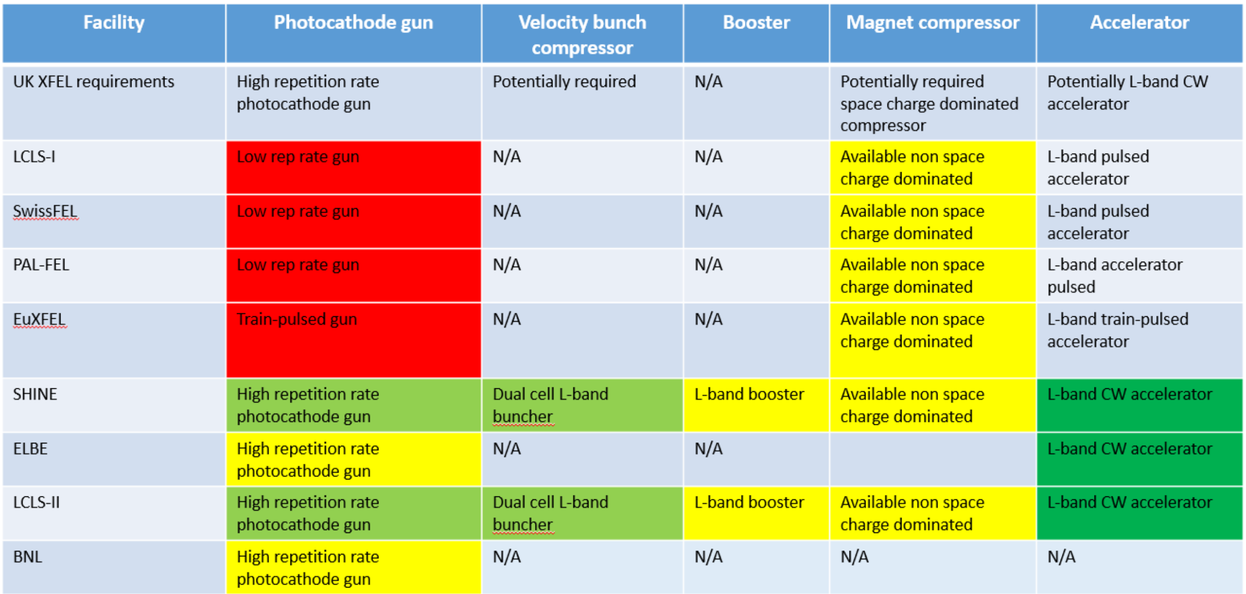
Facility (Location):	UK XFEL (STFC Daresbury Laboratory)
Electron Beam Energy (E):	8 GeV
Energy Spread (σ_γ):	$\leq 1 \times 10^{-4}$ [13]
Bunch Charge (I_{bunch}):	300 pC
Peak Current (I_{pk}):	3 kA [13]
Repetition Rate (f_{bunch}):	1 MHz (or more)
Average Current(I_{ave}):	0.3 mA
Normalised Emittance (ε_n):	$\leq$ 0.1 mm–mrad [13]

Table 1: Design specifications for the UK XFEL and gun/injector requirements.

3 High–Brightness Electron Injectors

There are a number of facilities around the world with high–brightness electron sources which are currently operational or in advanced stages of planning. These are summarised in Fig. 1.

The sources for LCLS–I, SwissFEL, PAL–FEL and the EuXFEL do not meet the repetition rate specification for the UK XFEL, so are not considered in this review. The LCLS-II and SHINE both meet the baseline specification for the UK XFEL, while aspects of both the ELBE and BNL injectors meet UK XFEL specifications, but they fail to meet all criteria.



Facility	Photocathode gun	Velocity bunch compressor	Booster	Magnet compressor	Accelerator
UK XFEL requirements	High repetition rate photocathode gun	Potentially required	N/A	Potentially required space charge dominated compressor	Potentially L-band CW accelerator
LCLS-I	Low rep rate gun	N/A	N/A	Available non space charge dominated	L-band pulsed accelerator
SwissFEL	Low rep rate gun	N/A	N/A	Available non space charge dominated	L-band pulsed accelerator
PAL-FEL	Low rep rate gun	N/A	N/A	Available non space charge dominated	L-band accelerator pulsed
EuXFEL	Train-pulsed gun	N/A	N/A	Available non space charge dominated	L-band train-pulsed accelerator
SHINE	High repetition rate photocathode gun	Dual cell L-band buncher	L-band booster	Available non space charge dominated	L-band CW accelerator
ELBE	High repetition rate photocathode gun	N/A	N/A		L-band CW accelerator
LCLS-II	High repetition rate photocathode gun	Dual cell L-band buncher	L-band booster	Available non space charge dominated	L-band CW accelerator
BNL	High repetition rate photocathode gun	N/A	N/A	N/A	N/A

Figure 1: Overview of worldwide high–brightness electron injectors.

4 LCLS–II: the Linac Coherent Light Source II at SLAC (USA)

Facility (Location):	LCLS–II (Stanford, CA, USA)
Gun Technology:	QWR NCRF @ 185.7 MHz [15] (7$^{\text{th}}$ sub–harmonic of main 1.3 GHz linac)
Field Gradient on Photocathode:	17.5 - 19.5 MV/m [15]
Drive Laser Technology:	Fibre Osc. + Amp (50 W @ 1030 nm) [16]
Drive Laser Pulse Length:	Gaussian, 20 – 60 ps FWHM [15, 17] @ 0.3 μJ/pulse [18]
Cathode Type:	Cs$_2$Te on an INFN–Type plug
Illumination Wavelength:	257.5 nm [16]
Typical QE @ Wavelength:	$>$0.5 % @ 257.5 nm [15, 16, 19]
MTE @ Wavelength:	??
Bunch Charge:	20 - 100 pC
Bunch Length:	$<$3.4 ps RMS [15]
Photons/Bunch:	??
Bunch Repetition Rate:	0.929 MHz
Average Beam Current:	0.03 mA [15]
Gun Energy ∣ Injector Energy:	650 – 750 keV ∣ $>$90 MeV [15], 80 – 90 MeV [18]
Beam Emittance @ Bunch Charge (Energy):	$<$0.5 μm @ 50 - 100 pC (?? MeV) [15]
Energy Spread:	??

Table 2: Summary of LCLS–II XFEL injector measured performance.

The LCLS-II injector is based on the Advanced Photoinjector Experiment (APEX) gun proposed in 2006 and developed at the Lawrence Berkeley National Laboratory [14]. It provides a solution to the high–brightness + high–repetition rate challenge by combining a normal-conducting cavity operating in the VHF region at continuous wave with a high QE cathode whose emission is accelerated to a moderate energy over a $\frac{1}{4}$RF wavelength. The unique design achieves the required XHV vacuum levels by placing the RF resonator inside a vacuum vessel populated with NEG pumping modules, with slots cut into the resonator which are substantially shorter than the RF wavelength thereby avoiding breakdown. Dark current is recognised as an issue with this gun, believed to originate from the inner lip of the gun nose cone [18]. Operation at reduced gradient minimises the dark current, with up to 95 % removed through collimation.

LCLS-II HE will see development of a new low emittance injector (LEI) based on an SRF QWR gun, which is anticipated to increase the cathode field to 30 MV/m and thus the beam energy to 1.8 MeV. The cathode is likely to be a bi–alkali (Cs$_3$Sb or a Cs$_3$Sb:Na$_2$KSb hybrid) with a photocathode exchange mechanism which is currently under development in a collaboration with HZDR.

5 SHINE: the Shanghai HIgh repetition rate XFEL aNd Extreme light facility (China)

Facility (Location):	SHINE (Shanghai, China)
Gun Technology:	QWR NCRF @ 216.67 MHz (6th sub–harmonic of main 1.3 GHz linac)
Field Gradient on Photocathode:	28 MV/m [20]
Drive Laser Technology:	??
Drive Laser Pulse Length:	??
Cathode Type:	Cs_2Te ∣ 'green' planned [20]
Illumination Wavelength:	??
Typical QE @ Wavelength:	??
MTE @ Wavelength:	??
Bunch Charge:	100 pC [21] ∣ 20 – 300 pC [22]
Bunch Length:	< 10 fs [23]
Photons/Bunch:	$\sim 10^{12}$ [23]
Bunch Repetition Rate:	1 MHz (implied, but not stated)
Average Beam Current:	?? mA
Gun Energy ∣ Injector Energy:	800 keV [20] ∣ 30 MeV
Bunch Charge ∣ Prj. Emittance ∣ Slc. Emittance ∣ Length:	10 pC ∣ 0.16 μm ∣ 0.15 μm ∣ 0.49 mm [20]
	50 pC ∣ 0.41 μm ∣ 0.38 μm ∣ 1.15 mm
	100 pC ∣ 0.85 μm ∣ 0.72 μm ∣ 1.44 mm
Beam Emittance @ Bunch Charge (Energy):	See Above
Energy Spread:	??

Table 3: Summary SHINE XFEL injector measured performance

Yingchao Du gave an update [22] at the 2023 US P3 workshop on the history and latest performance of the SHINE gun development, with the following key points. More than 30 guns were manufactured for the SHINE project by Tsinghua University, with 3 of these progressed through to a complete gun assembly. Operation at 216.7 MHz (1.3 GHz / 6) offers a higher cathode surface field up to 30 MV/m, but this also increases dark current. An alternate cavity resonant at 162 MHz (1.3 GHz / 8) is also compatible with the SHINE timing system. Multipacting has been an issue when the cathode field is < 16 MV/m. Gun operation has been restricted by an RF power limit of < 100 kW. A maximum temperature rise of 40 °C was observed at an RF power level of 90 kW, which caused a resonance shift of $\Delta f < 80$ kHz. the cavity quality factor is within 5 % of the design parameter.

6 HZDR: Helmholtz–Zentrum at Dresden, Rossendorf (Germany)

Facility (Location): ELBE (Rossendorf, Germany)
Gun Technology: 3.5 Cell SRF @ 1.3 GHz (Gun II) [25]
Field Gradient on Photocathode: 14.5 MV/m
Drive Laser Technology: Mode–locked Nd:glass @ 52 MHz
Drive Laser Pulse Length: Gaussian, 3 – 5 ps FWHM
Cathode Type: Mg
Illumination Wavelength: 257.5 nm
Typical QE @ Wavelength): 0.1 – 0.3 % @ 257.5 nm
MTE @ Wavelength: ??
Bunch Charge: 0 – 300 pC
Bunch Length: ??
Photons/Bunch: ??
Bunch Repetition Rate: 10 – 500 kHz | 13 MHz
Average Beam Current: $\leq 30\mu$A * [25]
Gun Energy | Injector Energy: 4.0 MeV | N/A
Beam Emittance @ Bunch Charge (Energy): 2 – 15 μm RMS * [25]
Energy Spread: 5 – 25 keV RMS * [25]

Table 4: Summary of design parameters for the ELBE injector at HZDR.
* Measurements taken with bunch charge of 200 pC [25]

This is an SRF gun with a photocathode exchange system, and so has operated with a number of different photocathode types including metals and semiconductors. The photocathode puck design differs from the INFN ‘standard’ due to the super–conducting nature of this gun.

The HZDR two-channel drive laser system for Gun-II was developed by the Max Born Institute, and provides a high level of flexibility with its range of repetition rates. The Nd:glass master oscillator generates a 52 MHz pulse train which is boosted by a regenerative amplifier in the 500 kHz mode or a fibre amplifier in the 13 MHz mode. Finally, a power amplifier boosts either mode and delivers this to the wavelength conversion stage which converts the IR to UV. Due to the non–linear nature of the wavelength conversion process, this stage is believed to be the source of instabilities in the final UV output beam.

7 Research Instruments, Lighthouse Project (Germany)

Facility (Location):	Research Instruments (Germany) for the Institut National des radio éléments (Belgium)
Gun Technology:	2 × 350 kV DC Photocathode Guns [26]
Field Gradient on Photocathode:	??
Drive Laser Technology:	??
Drive Laser Pulse Length:	??
Cathode Type:	CsK_2Sb
Illumination Wavelength:	520 nm
Typical QE @ Wavelength):	4 – 7 % @ 520 nm
MTE @ Wavelength:	??
Bunch Charge:	30 pC
Bunch Length:	20 ps
Photons/Bunch:	??
Bunch Repetition Rate:	1.3 GHz
Average Beam Current:	40 mA
Gun Energy | Injector Energy:	350 keV | 75 MeV
Beam Emittance @ Bunch Charge (Energy):	??
Energy Spread:	??

Table 5: Summary of design parameters for the Lighthouse Project injector.

The Lighthouse Project involves the development of an industrial accelerator for operation 23/7 in the production of radionucleotides through the irradiation of ^{100}Mo. The requirement for high beam current has necessitated the use of parallel DC photocathode guns using a bi–alkali photocathode, delivering a 350 keV beam into a series of 5 × CBETA class SRF accelerating modules to generate a final beam of 75 MeV. The gun technology does not match that planned for the UK XFEL, but the use of a bi–alkali photocathode and particularly the development of a repeatable photocathode preparation process is both notable and relevant.

8 Summary and Recommendations

SLAC and SHINE have both demonstrated photoinjector guns acheiving high repetition rate around 1 MHz with bunch charges up to 100 pC using Cs_2Te photocathodes, and this is close to the design specifications for the UK XFEL. The SLAC design for the LCLS-II [15] which has evolved over nearly two decades from the LBNL APEX gun has gained traction, with the NCRF VHF design also having been applied in several variations by Tsinghua University for the SHINE project [22].

Both of these guns currently use Cs_2Te photocathodes to generate their electron beam. Cs_2Te is a robust photocathode material, and its selection for both the LCLS–II and SHINE facilities is testament to the level of understanding and 'trust' ascribed to it by the accelerator community. Cs_2Te has demonstrated reliable operation with high levels of QE for long periods of operation, with both DESY and CERN having documented the extended use of Cs_2Te photocathodes, CERN for more than 1 year and DESY for more than 3 years with an integrated charge extraction exceeding 30 C.

However, the generation of sufficient UV photons ($\sim$ 266 nm) to illuminate the photocathode and extract a MHz pulse train of 300 pC electron bunches equating to a beam current of 0.3 mA (UK XFEL specification) would require a significant laser installation. This would leave little headroom for the inevitable laser system performance (power) deterioration, nor for the application of transverse and longitudinal laser pulse shaping which are recognised as being essential to minimise beam emittance, particularly in the generation of such high–charge electron bunches.

> ASTeC have demonstrated the ability to manufacture Cs_2Te photocathodes with QE in the 5 % regime, with the expectation that the QE levels will increase to between 10 and 12 % in the near future. Given the availability of suitable MHz-class UV drive laser systems, the use of Cs_2Te photocathodes is a viable current option for the UK XFEL.

Both SLAC and SHINE plan to test bi–alkali photocathodes which photoemit at green wavelengths ($\sim$ 532 nm), thus reducing the IR power requirement in the laser system, and potentially increasing drive laser beam stability due to the need to carry out only a single stage of frequency doubling. SLAC have stated that they expect to demonstrate this by 2027, while SHINE have not indicated a target date at this time. A complicating factor in the use of bi–alkali cathodes is their sensitivity to contamination and the consequent need to operate at extreme high vacuum (XHV) levels in the 10^{-11} mbar regime. Both SLAC and SHINE acknowledge that an improvement in their respective vacuum conditions is necessary for the successful deployment of this technology.

There are a range of bi–alkali cathode options, the most common within the accelerator community being Cs_3Sb, CsK_2Sb and Na_2KSb. ASTeC are at the beginning of a collaboration with HZB focusing on the growth and characterisation of Na_2KSb photocathodes, this choice having been made on the basis that the avoidance of a Cs-containing photocathode is preferable given its known affinity to react with oxygen–containing compounds and thus alter the photocathode chemistry, potentially impacting the energy spread of the photoemitted electrons (and emittance) and degrading the operational lifetime. Na_2KSb is therefore considered to be a more stable bi–alkali photocathode option. Laboratories in the USA are investigating the use of Cs_3Sb as a photocathode electron source.

ASTeC plan to develop a bi–alkali photocathode capability in the next 2 to 3 years, and are actively recruiting a Ph.D. research student to realise this goal. This programme of work is likely to start in September 2024, and will involve expanding the current Cs_2Te photocathode deposition system with additional sources to deposit sodium, potassium and antimony. The use of Cs_3Sb will remain an equally viable option for ASTeC, should progress in this technology be demonstrated elsewhere.

> ASTeC expect to demonstrate the ability to reproducibly manufacture bi–alkali photocathodes within 3 years with QEs in the 4 – 8 % range under illumination at 532 nm. These are a viable and attractive future option for the UK XFEL.

The use of a bi–alkali photocathode further simplifies the necessary drive laser technology, and creates ample capacity within the laser system for the application of sophisticated transverse and longitudinal beam shaping methods, thereby minimising electron beam emittance. Use of this technology also reduces the level of laser pulse amplitude instability which is introduced by having two stages of frequency–doubling, and removes the need to work with UV beams and the cumulative damage they cause to what are often expensive and inaccessible optics.

While the use of Cs_2Te as a high efficiency, high brightness, high repetition rate photocathode is possible at this time, the use of Na_2KSb (or Cs_3Sb) is preferable in several ways, and should be a viable option in due course given the likely timescale for the development of a UK XFEL.

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