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Ångström Laser

Synopsis: This report briefly summarizes the results of a design study of a compact coherent X-ray source based on superconducting (SC) accelerator technology. The X-ray source is envisioned to provide X-ray scientists at Uppsala University (UU) with high repetition rate femtosecond flashes of laser-like X-ray radiation for studying transient states of novel materials, biological and chemical systems.

Science applications and requirements: The Department of Physics and Astronomy of UU is an active player in the field of time-resolved X-ray photoelectron spectroscopy and operates an in-house photoelectron spectroscopy beamline based on a high-harmonic generation (HHG) source. It is of a high practical interest to go beyond the energy range provided by the HHG source limited to about 100 eV. The new X-ray source has to cover the region of approximately 1-4 keV and also operate at a high repetition rate of around 100 kHz. The photon flux into 0.1 eV bandwidth must provide reasonable data acquisition times. Sub-ps time resolution is needed for pump-probe studies. The space charge of photoemitted electrons is one the limiting factors of the photoelectron spectroscopy method and a moderately high number of X-ray photons per shot is desired. Between 100 and 10 thousand of X-ray photons into *0.1 eV bandwidth* would be well suited for photoelectron spectroscopy. To avoid heat-related effects in the sample, the separation between the X-ray pulses must be larger than the typical relaxation time of the sample, which is of the order of one microsecond. Thus, for science applications, the best time structure of X-ray radiation is of that a train of evenly spaced X-ray pulses at 100 kHz.

Technology choice: *Free-Electron Laser (FEL) technology* allows producing X-ray radiation with the highest brightness among other laboratory X-ray technologies and we choose to use FEL technology to generate the required number of photons into 0.1 eV bandwidth. The required high-repetition rate of evenly spaced X-ray pulses calls for a continuous wave (CW) regime of the accelerator. Hence, *superconducting (SC) accelerator technology* is adopted to keep the accelerator compact by providing sufficiently high accelerating gradients in CW operation. The use of an ultra-short period laser undulator is currently the main strategy for the generation of X-ray pulses in the 1-4 keV range while having moderate requirements on the electron beam energy.

Phased approach: The complexity of the envisioned coherent X-ray source is very high and therefore we plan a two-stage approach: (i) an incoherent X-ray source based on the mechanism of Compton scattering and (ii) a coherent X-ray source based on coherent spontaneous undulator radiation from a pre-bunched electron beam with subsequent amplification of coherent radiation via the FEL mechanism. Below, we exemplify X-ray performance in the phase I and II assuming state-of-the-art parameters of an electron beam and an external laser. Then, we introduce a conceptual layout of the X-ray source and present the current status of our start-to-end (S2E) beam dynamics studies.

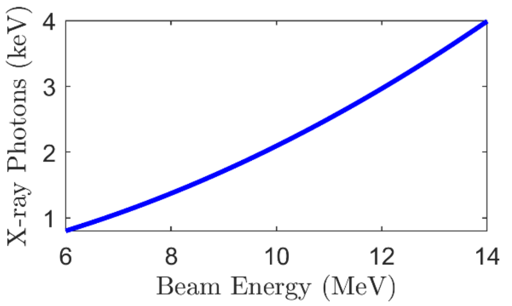

Fig. 1: Maximum energy of scattered photons vs. electron beam energy.

Phase I, Compton source: In a Compton source, a laser photon beam collides with a counterpropagating electron beam. The energy of backscattered photons is upshifted by a factor of $4\gamma^2$ for a head-on collision with γ being the energy of the electron beam in units of the rest mass. For relativistic electron beams and optical photon beams, the energy of the scattered photons lies in the X-ray spectral region. With recent progress of commercial lasers in the production of ps pulses on the sub-Joule level, the production of fs X-ray pulses through the *inverse Compton effect* becomes a viable option.

We consider a high-power OPCPA from TRUMPF: 50-mJ, 1-ps pulses peaked at 1 μm and reproduced at 100 kHz repetition rate [1]. This laser system is currently state-of-the-art but we note that even higher power versions are in development. Each optical pulse comprises approximately 300 cycles of light oscillations. The corresponding pulse bandwidth (BW) is around 0.3%.

The inverse Compton scattering of such laser pulses on an electron beam with an energy tunable from 6 to 14 MeV results in X-ray photons in the range from around 1 to 4 keV, see Fig. 1.

The parameters of the Compton source are estimated using the *model of spontaneous undulator radiation* for the effective equivalent magnetic undulator [2,3]. The results are presented in Table I. The electron bunch is assumed to be moderately compressed to provide the minimum broadening of Compton X-ray spectrum through the energy spread effect. The ponderomotive broadening is assumed to be compensated for by chirping the laser pulse. The natural broadening of on-axis radiation due to 3D effects [4] amounts to 0.42%. The analytically estimated number of X-ray photons at 1 nm into *0.1 eV bandwidth* is 780. This number can be tripled by increasing the laser pulse energy to 500 mJ while reducing the repetition rate to 10 kHz.

Table I: Target parameters of the Compton source. The electron bunch parameters are depicted in blue, the laser parameters in red, and the X-ray yield in black.

Electron beam parameters	electron bunch charge	Q_b	16	pC
	number of electrons	N_b	10^8	
	bunch energy	U_b	7.6	MeV
	relative energy spread	δ_γ	10^{-4}	
	rms bunch duration	τ_b	0.25	ps
	bunch emittance	ϵ_n	0.1	mm mrad
	rms bunch size	σ_b	3.5	um
	geometrical beta-function	β_g	2	mm
Laser beam parameters	laser wavelength	λ_L	1.0	um
	rms laser pulse duration	τ_L	1	ps
	rms laser beam size	σ_L	4.9	um
	Rayleigh length	z_R	0.3	mm
	laser pulse energy	$\mathcal{E}_L$	50	mJ
	undulator parameter	$\mathcal{K}$	0.14	
	laser rep. rate	f_L	100	kHz
X-ray yield	radiation wavelength	λ_r	1	nm
	rms X-ray pulse duration	τ_X	0.25	ps
	rms X-ray beam size	σ_X	3.5	um
	rms X-ray beam divergence	$\sigma_{X'}$	0.4	mrad
	X-ray photons/shot/0.01%BW	$N_{ph,0.01\%}$	780	
	X-ray photons/second/0.01%BW	$\mathcal{F}_{0.01\%}$	7.8 10^7	

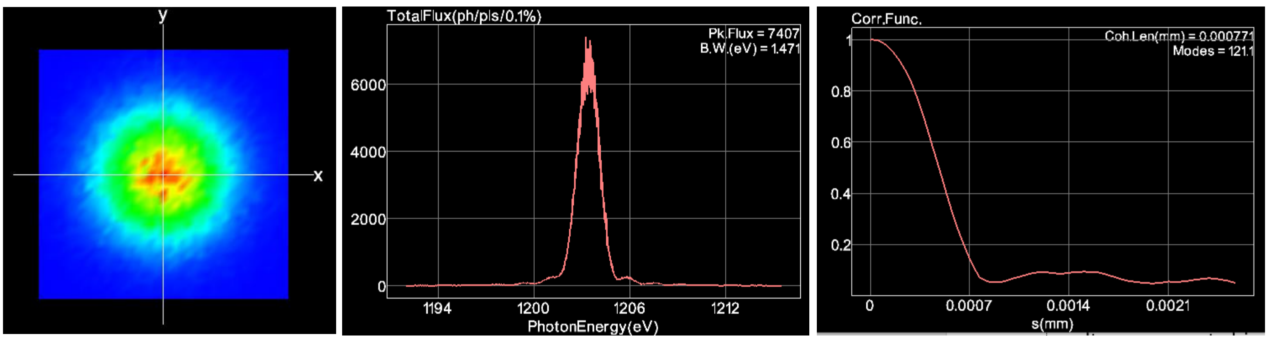

Fig. 2: Simulation results for the Compton source using the Tanaka code Simplex [5]. From left to right: the power density averaged over the pulse as a function of transverse coordinates, the photon flux per shot vs photon energy, and the temporal correlation functions of the 1st order as a function of distance.

For crosschecking, numerical simulations with the simulation code Simplex [5] were performed and the results are presented in Fig. 2. The laser undulator is treated as an effective magnetic undulator. The photon flux per shot into 0.1 eV bandwidth is around 700 photons which is consistent with the analytical estimate. Note that transverse profile of the average power density has a speckle pattern due to the stochastic nature of spontaneous radiation. The power density distribution changes from shot to shot. The divergence of the X-ray beam is large, 0.4 mrad, which makes X-ray transport challenging.

Phase II, coherent X-ray source: In the second phase, the electron beam will be prebunched on the nanometer scale to provide strong coherent spontaneous undulator radiation with subsequent exponential amplification via the FEL mechanism. Our main present approach for nanometer bunching relies on a recently proposed idea of electron beam nanopatterning in the transverse coordinate space via electron diffraction on a perforated crystal, and a subsequent emittance exchange [6,7,8]. Start-to-end beam dynamics simulations in the accelerator are presently ongoing but the bunch distribution is not tracked yet all the way to the laser undulator. Hence, the X-ray source performance is estimated for a model electron bunch assuming a bunching factor of 0.4. The results are summarized in the Table II. Over 10000 photons into 0.1 eV per shot are expected to be produced.

Table II: Target parameters of the coherent X-ray source.

Electron beam parameters	electron bunch charge	Q_b	0.8	pC
	number of electrons	N_b	$5\ 10^6$	
	bunch energy	U_b	7.6	MeV
	relative energy spread	δ_γ	10^{-4}	
	rms bunch duration	τ_b	50	fs
	bunch emittance	ϵ_n	0.03	mm mrad
	rms bunch size	σ_b	2	um
	geometrical beta-function	β_g	2	mm
Laser beam parameters	laser wavelength	λ_L	1.0	um
	rms laser pulse duration	τ_L	1000	fs
	rms laser beam size	σ_L	4.9	um
	Rayleigh length	z_R	0.3	mm
	laser pulse energy	$\mathcal{E}_L$	50	mJ
	undulator parameter	$\mathcal{K}$	0.14	
	laser rep. rate	f_L	100	kHz
X-ray yield	radiation wavelength	λ_r	1	nm
	X-ray pulse duration	τ_X	50	fs
	rms X-ray beam size	σ_X	1.5	um
	rms X-ray beam divergence	$\sigma_{X'}$	75	urad
	X-ray photons/shot/0.01%BW	$N_{ph,0.01\%}$	$3\ 10^4$	
	X-ray photons/second/0.01%BW	$\mathcal{F}_{0.01\%}$	$3\ 10^9$	

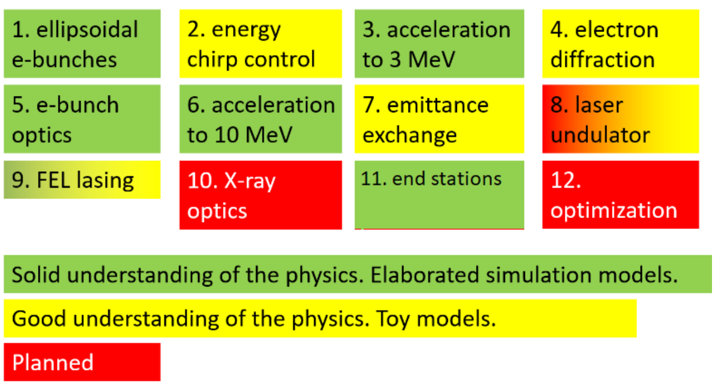

Fig. 3: High-level conceptual layout of the coherent X-ray source and a present status of S2E simulations.

In this approach, we foresee two main risks: (i) degradation of the beam emittance in the low-energy part of the accelerator due to space-charge forces, and (ii) degradation of the bunching factor in the emittance exchange part because of nonlinear forces in realistic accelerator components.

X-ray source conceptual layout: Figure 3 shows a conceptual layout of the coherent X-ray source. The Compton source uses the same layout but some elements such as nanopatterning and emittance exchange are inactive. Each block of the layout represents a physical process and is composed of many technical systems. In simulations, the block is an independent unit based on a combination of software tools. The blocks can be independently assembled into a required simulation configuration:

1. Ellipsoidal electron bunches with a charge of 1.6 pC for the coherent source (16 pC for the Compton source) and a transverse emittance of 30 nm (100 nm) are produced with an energy of around 0.4 MeV. The electron gun is based on a normal conducting CW RF cavity at 325 MHz.
2. A third harmonic cavity is used to control the longitudinal phase space of the beam.
3. A SC booster at 1.3 GHz accelerates the beam to around 3 MeV to reduce the space-charge effect. The booster is also used for velocity bunching.
4. A perforated crystal, as proposed in [6], introduces a periodic modulation in the transverse phase space of the beam.
5. As the beam propagates in space, the modulation in the phase space is converted into a density modulation in the physical space and the beam splits into two. One of the beams is steered further into the accelerator whereas the other one is used for electron diagnostic.
6. A 1.3 GHz SC elliptical cavity brings the beam to the nominal voltage.
7. An emittance exchange line with compensation for nonlinear forces [7] is used to rotate the beam in the physical space and swap the transverse emittance with the longitudinal one. The exchange line makes use of a SC deflector cavity and a SC correction cavity. Both cavities are at 1.3 GHz.
8. Laser pulses from a high-power laser amplifier, like TRUMPF Dira, are focused into a tight spot for creating an optical undulator for the electron beam.
9. The electron beam prebunched on the nanometer scale emits strong coherent spontaneous undulator radiation which is amplified further in an exponential fashion via the FEL mechanism.
10. An X-ray beamline is used to reduce further the bandwidth of the X-ray beam and focus it onto the target. A double-crystal monochromator and Kirkpatrick-Baez mirrors are assumed.
11. The end station is intended to support both gaseous and solid samples.
12. At the end, we plan to perform multi-objective optimization of the complete simulation model.

End station: Photoemission spectroscopy in the vacuum ultraviolet to X-ray spectral range has become one of the central tools at synchrotron light sources. Currently, spectrometers for photoemission studies are mainly based on hemispherical electrostatic electron kinetic energy analysis where the relatively low photon count per pulse avoids electronic space charge limiting detection. It is interesting to note that a spin-off company from UU has developed into a market leader for such spectrometers. Here, we will use a radically different approach based on energy analysis via measuring *the time of flight* (ToF) of photoemitted electrons. This kind of spectrometer has been pioneered by Gerd Schönhense (Uni Mainz) and several instruments developed and build by his team are in operation at synchrotron sources (BESSY II, PETRA III) and free electron lasers (FLASH and in the near future EU-XFEL). It consists of electron optics that can image the full angular distribution of X-ray photoelectrons combined with ToF analysis (3D recording scheme) [9,10]. This enables an efficient detection of nearly all photoelectrons, in contrast to hemispherical energy analysis where only a section of the k-distribution along one line is detected simultaneously (2D scheme). The important consequence is that a relatively low X-ray flux from pulsed sources (typically 10^8 photons/sec) is sufficient to obtain high-quality spectra [10]. This so-called momentum microscope is therefore optimally suited for our proposed Ångstrom Laser, whereas at free electron lasers its operation is only possible after severely attenuating the intense X-ray beam.

Space considerations: The X-ray source requires a SC accelerator for CW operation at 100 kHz. The FREIA Laboratory at the Department of Physics and Astronomy of UU is well equipped to host and operate the SC accelerator for the X-ray source. The FREIA Laboratory of around 1 000 m^2 is dedicated to (high-power) characterization of SC cavities and SC magnets. It houses a cryogenic system with a He liquefier, several high-power RF sources at 352 MHz, a horizontal and a vertical cryostat, and electronics for stabilizing accelerating fields in SC cavities. This is typically the infrastructure required for the SC accelerator. Figure 4 shows an area potentially available for the X-ray source along with a very preliminary layout of technical systems of the X-ray source. This area contains 3 bunkers which can be reconfigured to fit the X-ray source. The horizontal cryostat can be re-used for two SC cavities.

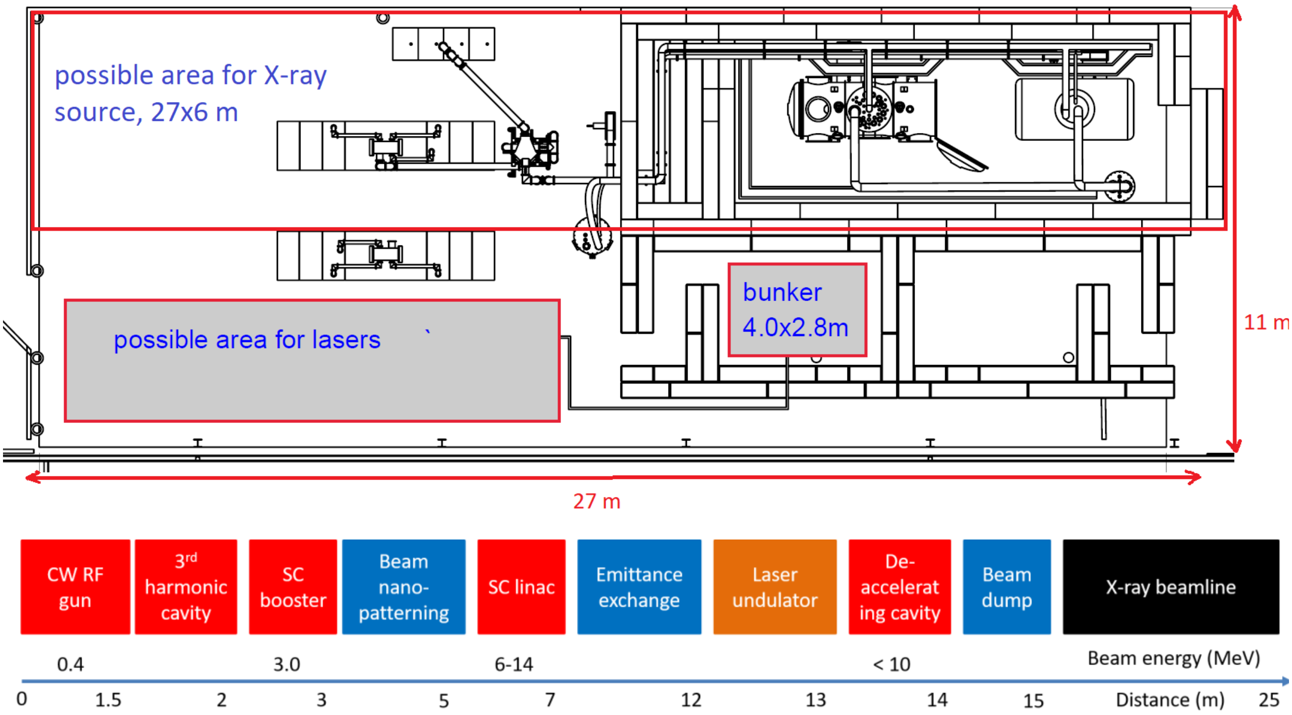

Fig. 4: Top: sketch of the total area for accelerator experiments at the FREIA laboratory. The maximum possible area for the X-ray source is 27 x 6 m. An additional area for a high-power laser along with a test bunker area are also available. Bottom: a preliminary layout of the X-ray source components.

Summary: The proposed compact X-ray source occupies a unique niche among HHG, FEL and synchrotron sources in terms of the repetition rate, pulse duration and photon energy range. Our compact X-ray source can be directly compared only to femtosecond (fs) slicing sources at synchrotrons but outperforms the latter by 3 orders of magnitude in terms of photon flux even in the Phase I. For reference, the fs slicing source at PSI [11] delivers 4 10^4 photons into 0.01% BW in the range 4-14 keV whereas the fs slicing source at BESSY [12] produces 10^5 photons into 0.01% BW in the range 0.4-1.4 keV. Both slicing sources have proved to be instrumental for ultrafast X-ray science as reflected in corresponding PRL, Nature and Science publications. Clearly, the proposed compact and bright X-ray source would create bright perspectives for cutting-edge time-resolved X-ray science experiments at Uppsala University.

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