Inverse-Designed Narrowband THz Radiator for Ultrarelativistic Electrons

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ABSTRACT: THz radiation finds various applications in science and technology. Pump–probe experiments at free-electron lasers typically rely on THz radiation generated by optical rectification of ultrashort laser pulses in electro-optic crystals. A compact and cost-efficient alternative is offered by the Smith–Purcell effect: a charged particle beam passes a periodic structure and generates synchronous radiation. Here, we employ the technique of photonic inverse design to optimize a structure for Smith–Purcell radiation at a single wavelength from ultrarelativistic electrons. The resulting design is highly resonant and emits narrowbandly. Experiments with a 3D-printed model for a wavelength of 900 μm show coherent enhancement. The versatility of inverse design offers a simple adoption of the structure to other electron energies or radiation wavelengths. This approach could advance beam-based THz generation for a wide range of applications.

KEYWORDS: THz generation, Smith–Purcell radiation, inverse design, light–matter interaction, free-electron light sources

Sources of THz radiation are of interest for numerous applications, including wireless communication,1,2 electron acceleration,3–5 and biomedical and material science.5,7 Free-electron laser (FEL) facilities demand versatile THz sources for pump–probe experiments.9 Intense, broadband THz pulses up to sub-mJ pulse energy have been demonstrated using optical rectification of high-power femtosecond lasers in lithium niobate crystals.9,10 The Smith–Purcell effect11 offers a compact and cost-efficient alternative for the generation of beam-synchronous THz radiation at electron accelerators. This effect describes the emission of electromagnetic waves from a periodic metallic or dielectric structure excited by electrons moving parallel to its surface. The wavelength of Smith–Purcell radiation at an angle θ with respect to the electron beam follows:11

\[
\lambda = \frac{a}{m} \left( \frac{1}{\beta} - \cos \theta \right)
\]  

(1)

where β is the normalized velocity of the electrons, a is the periodicity of the structure, and m is the mode order. Smith–Purcell emission from regular metallic grating surfaces has been observed in numerous experiments, first using 300 keV electrons11 and later also using ultrarelativistic electrons.12,13 If electron pulses shorter than the emitted wavelength are used, the fields from individual electrons add coherently, and the radiated energy scales quadratically with the bunch charge.14 The typically used single-sided gratings emit a broadband spectrum,15 which is dispersed by the Smith–Purcell relation (eq 1). To enhance emission at single frequencies, a concept called orotron uses a metallic mirror above the grating to form a resonator.16,17 Dielectrics can sustain fields 1–2 orders of magnitude larger than metals18 and are therefore an attractive material for strong Smith–Purcell interactions.

Inverse design is a computational technique that has been successfully employed to advance integrated photonics.19 Algorithms to discover optical structures fulfilling desired functional characteristics are creating a plethora of novel subwavelength geometries; applications include wavelength-dependent beam splitters20,21 and couplers,21 as well as dielectric laser accelerators.22

RESULTS

The goal of our inverse design optimization was a narrowband dielectric Smith–Purcell radiator for ultrarelativistic electrons (E = 3.2 GeV, γ ≈ 6000). To simplify the collection of the THz radiation, a periodicity of a = λ was chosen, resulting in an emission perpendicular to the electron propagation direction, θ = 90°. The optimization was based on a 2D finite-difference frequency-domain (FDFD) simulation of a single unit cell of the grating (Figure 1a). Periodic boundaries in direction of the electron propagation ensure the desired periodicity, and perfectly matched layers in the transverse x-direction emulate free space. The design region extends 4.5 mm to each side of a 150 μm wide vacuum channel, large enough to facilitate the full transmission of the electron beam with a

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width of $\sigma = 30 \, \mu m$ (RMS). The electric current spectral density $J(x, y, \omega)$ of a single electron bunch acts here as the source term of our simulation and is given by

$$J(x, y, \omega) = \frac{q}{2\pi} \left( \frac{2\pi\sigma^2}{x} \right)^{-1/2} e^{-x^2/2\sigma^2} e^{-\omega^2/\omega_0^2}$$

with the electron wavevector $k_y = 2\pi/\beta \lambda$ and the line charge density $q$. The absolute value of $q$ is irrelevant for the optimization, but rough agreement with 3D simulations is found by choosing $q \sim Q/d$, where $Q$ is the bunch charge and $d$ the charge-structure distance.\(^{23}\)

The optimization problem was to find a design (parametrized by the variable $\phi$) that maximizes the radiation to both sides of the grating. Exploiting the full symmetry of the double-sided, perpendicular emission process, we enforced mirror and point symmetry with respect to the center of a unit cell of the grating. The design is defined by its relative permittivity $\varepsilon(x, y, \phi)$ and can only take the two values of vacuum, $\varepsilon = 1$, or the structure material, $\varepsilon = 2.79$. For simplicity, we neglected the small imaginary part $\varepsilon'' = 0.08$ of the material.\(^{24}\)

The objective function $G$, quantifying the performance of a design $\phi$, is given by the line integral of the Poynting vector $S(x, y)$ outside the design region:

$$G(\phi) = \int_{x_S}^{a} S(x, y) dy$$

The optimization problem can then be stated as

$$\max_{\phi} \quad G(\phi) \quad \text{subject to} \quad \nabla \times E = -i\omega \mu B \quad \text{and} \quad \nabla \times \varepsilon(\phi)^{-1} \nabla \times H = \nabla \times \varepsilon(\phi)^{-1} J$$

The design obtained from the gradient-based technique of adaptive moment estimation (Adam)$^{25}$ is depicted in Figure 1b. The structure features two rows of pillars, shifted by half a period with respect to each other. The rows of pillars are followed by three slabs on each side, which can be easily
identified as distributed Bragg reflectors forming a microresonator around the electron channel. The channel width is 272 μm, even larger than the initially defined clearance of 150 μm. These slabs exhibit grooves, which perhaps act as a grating as well as a reflector. We note that these features are good examples of the superiority of inverse design over intuition-based designs.

To fabricate the geometry obtained with inverse design, we used an additive manufacturing process for poly(methyl methacrylate) (PMMA). A stereolithography device, featuring a resolution of 140 μm, is capable of reproducing the structure with subwavelength accuracy. The so-obtained structure is 6 mm high and 45 mm long (Figure 1d). The holder of the structure was manufactured together with the structure, and filaments connect the pillars and slabs on top of the structure for increased mechanical stability. We selected the Formlabs High Temperature Resin as a material for this study due to its excellent vacuum compatibility after curing in a heated vacuum chamber.24 Afterward, the fabricated Smith–Purcell radiator was inserted into the ACHIP experimental chamber20 at SwissFEL27 (Figure 2a). The photoemitted electron bunch is accelerated to an energy of 3.2 GeV with the normal-conducting radio frequency accelerator at SwissFEL. A two-stage compression scheme using magnetic chicanes is conducting a resolution of 140 μm, the FDTD simulation reproduced the measured spectrum much better. We also note that potential absorption losses in the structure can reduce its quality factor and broaden the radiation spectrum. Due to the small contribution from ε″ ≈ 0.08,24 absorption effects were not considered here but would dominate at higher quality factors.

We drove the structure with electron bunches with a duration of approximately 30 fs (RMS), which is much shorter than the resonant wavelength corresponding to a period of 3 ps. Hence, we expect to see the coherent addition of radiated fields. To experimentally verify this, we varied the bunch charge. Figure 4 shows the detected pulse energy for six bunch charge settings ranging from 0 pC to 11.8 pC. The scaling is well approximated by a quadratic fit, which confirms the expected coherent enhancement of the THz pulse energy.14 We observe a slight deviation for the highest charge measurement from the quadratic fit, which might be a result of detector saturation (see Methods). We note that the quadratic scaling would enable THz pulse energies orders of magnitude larger by driving the structure at higher bunch charges.

The THz pulse emitted perpendicular to the Smith-Purcell radiator possesses a pulse-front tilt of close to 45° since it is driven by ultrarelativistic electrons. Depending on the length of the radiator and the application, the tilt can be compensated for with a diffraction grating.

During and after our experiments, the structure did not show any signs of performance degradation or visible damage. It was
used continuously for eight hours with a bunch charge of approximately 10 pC at a pulse repetition rate of 1 Hz.

**CONCLUSION**

The here-presented beam-synchronous radiation source can be added to the beamline of an FEL to enrich capabilities for pump–probe experiments. For ultrarelativistic electrons, a second beamline may be used to compensate for the longer path length of the THz pulse. X-rays are generated in the undulators of an FEL. (b) For subrelativistic electrons, the generated THz pulse is delayed to achieve simultaneous arrival of electron and THz radiation. (c) The structure becomes a tunable light source if the periodicity changes along the invariant direction; exemplified with a rectangular grating.

**METHODS**

**Structure Parametrization.** Our inverse design process was carried out with an open-source Python package\(^\text{25}\) suitable for 2D-FDFD gradient-based optimizations\(^\text{25}\) of the chosen objective function \(G(\phi)\) with respect to the design parameter \(\phi\). A key step lies in the parametrization of the structure \(\epsilon(\phi)\) through the variable \(\phi\) in a way that ensures robust convergence of the algorithm and fabricability of the final design. In the most rudimentary case, \(\epsilon(x, y) = \phi(x, y)\) is a two-dimensional array with entries \(\epsilon \in [1, 2.79]\) for each pixel of the design area. Instead of setting bounds on the values of \(\phi\), we leave \(\phi\) unbounded and apply a sigmoid function of the shape

\[
\epsilon(x, y) = \epsilon_{\min} + \left(\epsilon_{\max} - \epsilon_{\min}\right) \frac{1}{2} \left(1 + \tanh(\alpha \phi(x, y))\right)
\]

where large values of \(\alpha\) yield a close-to-binary design with few values between \(\epsilon_{\min} = 1\) and \(\epsilon_{\max} = 2.79\). To avoid small or sharp features in the final design, we convolved \(\phi(x, y)\) with a uniform 2D circular kernel with radius 60 \(\mu m\) before projection onto the sigmoid function \(\tanh(\alpha \phi)\) with the convolved design parameter \(\phi\). By increasing \(\alpha\) from 20 to 1000 as the optimization progresses, we found improved convergence. We further accelerated convergence by applying mirror and point symmetry with respect to the center of a unit cell of the grating, which reduces the parameter space by a factor of 4. An exemplary design evolution is shown in Figure 6.

**Ultrarelativistic Optimization.** The simulation of ultrarelativistic electrons poses challenges that have so far prevented inverse design in this regime.\(^\text{30,31}\) Here, we report on two main challenges. First, the electron velocity is close to the speed of light \((\beta = 0.9999999885\) for \(E = 3.2\) GeV\), which requires a high mesh resolution. If the numerical error is too large due to a low mesh resolution, the simulation may not be able to distinguish between \(\beta < 1\) and \(\beta > 1\). In that case, the simulation could show Cherenkov radiation in vacuum instead of Smith–Purcell radiation.

Not only does a higher mesh resolution require more computational memory and time, but it may also hamper the inverse design optimization if the number of design parameters becomes too large. Hence, we parametrized our structures at a low resolution (mesh spacing \(\lambda/30\)), which is still above the fabrication accuracy of \(\lambda/5\), and computed the fields at a high resolution (mesh spacing \(\lambda/150\)).

The second difficulty arises from the long-range evanescent waves of ultrarelativistic electrons. The spectral density of the electric field of a line charge decays with \(\exp(-\kappa |x|)\), where \(\kappa = 2\pi/|\beta \gamma \lambda|\), with \(\beta \approx 1\) and \(\gamma \approx 6000\) for \(E = 3.2\) GeV.\(^\text{34}\) This

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![Figure 5. Possible applications of the beam-driven THz source in pump–probe experiments. (a) For ultrarelativistic electrons, a second electron bunch may be used to compensate for the longer path length of the THz pulse. X-rays are generated in the undulators of the FEL (Figure 5a). Smith–Purcell radiation represents a cost-efficient alternative to the broadband generation of THz by optical rectification, which requires an external laser system and precise synchronization to the accelerator. Our inverse design approach to Smith–Purcell emitters can produce beam-synchronous narrowband THz radiation, which could propel pump–probe studies with THz excitations in solids, for instance, resonant control of strongly correlated electron systems, high-temperature superconductors, or vibrational modes of crystal lattices (phonons).\(^\text{29,28}\) Further improvement of our THz structure can be achieved by higher fabrication accuracy and the use of a fully 3D-optimized geometry with a higher quality factor, resulting in more narrowband emission and higher pulse energy. Moreover, the inverse design suite could be extended to composite structures of more than one material, which could provide extra stability for complicated 3D designs. In the case of highly resonant structures, materials with low absorption, for example, polytetrafluoroethylene (PTFE),\(^\text{24}\) are a necessity. The measured THz pulse energy can be increased by a factor of almost 300 by raising the driving bunch charge from the used 11.8 pC up to the 200 pC available at SwissFEL. Whether the currently used material can withstand such high fields and radiation remains to be investigated. Combining 3D optimization, longer structures, larger collection optics, and higher bunch charges will result in a THz pulse energy multiple orders of magnitude larger than observed in the presented experiment (0.6 pJ).

Our work naturally extends to the field of subrelativistic electrons. Here, simultaneous arrival of THz radiation and electron bunches is readily achieved by compensating for the higher velocity of the radiation with a longer path length (Figure 5b). Besides its application for pump–probe experiments, our structure can be more generally applied as a radiation source at wavelengths that are otherwise difficult to generate. An advantage lies in the tunability that arises from changing the periodicity, either by replacing the entire structure or using a design with variable periodicity (Figure 5c), or from tuning the electron velocity. For the visible to UV regime, the idea of a compact device with the electron source integrated on a nanofabricated chip has recently sparked interest.\(^\text{30,31}\)
means the evanescent waves will reach the boundaries of our simulation cell in the x-direction. Generalized perfectly matched layers (PMLs)\textsuperscript{15} are chosen, such that they can absorb both propagating and evanescent waves.

A detailed look at Figure 1b reveals that our implementation of generalized PMLs is not fully capable of absorbing evanescent waves. Hence, we make use of symmetry to further reduce the effect of evanescent waves at the boundaries of the simulation cell. Note that the evanescent electric field for $\beta \gg 1$ is almost entirely polarized along the transverse direction $x$. This means if the simulation cell is mirror symmetric with respect to the electron channel, antiperiodic boundaries can be applied after the PMLs to cancel out the effect of evanescent waves at the boundaries. This turned out to work well for us, although the structure is not mirror symmetric with respect to the electron axis.

Simulations. The 3D frequency-domain simulation was performed in COMSOL, based on the finite element method. The simulation cell, as shown in the lower right inset of Figure 1c, consists of a single unit cell of the grating, with a height of 4 mm and periodic boundaries along the electron propagation direction. An optional phase shift at the boundaries in longitudinal direction enables simulations for nonperiodic Smith-Purcell emission, $\lambda \neq a$. Perfectly matched layers are applied in all remaining, transverse directions. The electron beam ($E = 3.2$ GeV, $Q = e$) had a Gaussian shape of width $\sigma_x = \sigma_z = 50 \mu m$ in the transverse direction.

The 3D time-domain simulation of the full structure, as shown in Figure 1c with the connecting filaments at the top and bottom, was performed in CST Studio Suite 2021. A single electron bunch ($E = 3$ GeV) with Gaussian charge distribution was assumed. Its width in the transverse direction was $\sigma_x = 0.1$ mm and in the longitudinal direction $\sigma_z = 0.2$ mm with cutoff length 0.4 mm. The simulation was performed for a longer bunch length than the experimental bunch length due to computational resource limitations for smaller mesh cell resolutions. Nevertheless, we expect this approximation to yield a realistic emission spectrum, since the simulated bunch length is still substantially shorter than the central wavelength. A convergence test showed that a hexahedral mesh with a minimum cell size of 15 $\mu m$ was sufficient. To imitate free space, perfectly matched layers and open-space boundary conditions were applied, where a $\lambda/2$ thick layer of vacuum was added after the dielectric structure. The radiation spectrum was then obtained via far-field approximations at multiple frequencies.

Accelerator Setup. The experiments used 10 pC electron bunches from the 3.2 GeV Athos beamline of SwissFEL\textsuperscript{27} operated at a pulse repetition rate of 1 Hz to keep particle losses during alignment at a tolerable level. The standard bunch charge at SwissFEL is 200 pC at a repetition rate of 100 Hz. For the low charge working point, the aperture and intensity of the cathode laser are reduced. The normalized emittance of the electron beam with a charge of 9.5 pC was 110 nm rad in both planes and was measured with a quadrupole scan in the injector at a beam energy of 150 MeV.$^\text{36}$

For the experiment, we scanned the charge from 0 to 11.8 pC by adjusting the intensity of the cathode laser, which results in a slight emittance degradation and mismatch of the transverse beam parameters. This is due to charge density changes in the space charge dominated gun region. Nevertheless, the beam size remained small enough for full transmission through the THz Smith–Purcell cell.

A bunch length of 30 fs (RMS) was measured for similar machine settings in a separate shift with a transverse deflecting cavity (TDC) in the Aramis beamline of the accelerator. Therefore, we expect the longitudinal dimension of the electron beam at the ACHIP chamber to be on the order of 10 $\mu m$, almost 2 orders of magnitude shorter than the period of the structure and radiated wavelength.

The transverse beam size at the interaction point was 30 $\mu m$ in the horizontal and 40 $\mu m$ in the vertical direction (for a charge of 9.5 pC), as measured with a scintillating YAG screen imaged with an out-of-vacuum microscope onto a CCD camera. After position and angular alignment of the structure using an in-vacuum hexapod, the beam could be transmitted without substantial losses through the 272 $\mu m$ wide channel of the THz generating structure.

Structure Fabrication. The structure was fabricated with a commercial PMMA stereolithography device Formlabs Form 2. The resolution of the device is 140 $\mu m$, which provides subwavelength feature sizes for the geometry with a periodicity of 900 $\mu m$. The height of the structure (6 mm) was limited by the stability of the structure rods during the fabrication process. The high temperature resin used for this study can be heated to 235 °C. A sufficiently low outgassing rate for the installation at SwissFEL was achieved after baking the device for 5 h under vacuum conditions at 175 °C.\textsuperscript{24,25} Thanks to the rapid improvements in SLA technology and other free-form manufacturing techniques, the geometry could certainly be fabricated also at shorter wavelengths and higher resolution for future experiments. An increased manufacturing quality is required to achieve an even narrower emission bandwidth.

Michelson Interferometer and THz Detector. For the spectrum measurements, we installed a Michelson interfer-

Figure 6. Exemplary design evolution. Left to right: The first 100 steps of an exemplary inverse design optimization are shown above their respective objective value in relative units. Starting from a random design, the design evolves under stochastic gradient-based optimization. At multiple steps throughout the optimization, the design solution is disturbed by the addition of random noise and blurring of features, which tests the stability of the design and helps in exploring a larger design space. Such a procedure was repeated $\sim 50 \times$, each time yielding a different design depending on the initial randomized design (similar to particle swarm optimization). We then selected those design groups that gave best performance, stability, and fabricability (similar to supervised learning). Continuing the optimization from there and repeatedly disturbing the solution, a final design will have gone through more than 1000 steps of optimization before fabrication. The displayed structure evolution used slightly different optimization conditions than the design presented in this work.
The interferometer allowed us to measure the ranging from 0.1 to 1 mm. Translating one of the mirrors of TYDEX. It provides a splitting ratio of 54/46 for wavelengths high-resistivity interferometer autocorrelation, from which the power spectrum is obtained according to the Smith Terahertz radiation de window with about 50% transmission for the design wave-should be characterized with a calibrated THz source. We setup including absorption in cables and the vacuum window bunker. For absolute pulse energy measurements, the detector long coaxial cable to an oscilloscope outside of the accelerator detector. The signal from the detector is transmitted via a 20 m detector. Around the orthogonal direction (θ = 90°), the accepted bandwidth covers the measured spectrum (Figure 3). We calculated the acceptance with ray tracing including the size of the emitting structure and the apertures of the collimating lens (25 mm) and the detector (12 mm). A Schottky diode (ACST, Type 3DL 12C LS2500 A2) was used as THz detector, sensitive from 300 to 4000 μm. The manufacturer indicates a responsivity of 120 V/W at 900 μm, which we used to estimate the energy deposited on the detector. The signal from the detector is transmitted via a 20 m long coaxial cable to an oscilloscope outside of the accelerator bunker. For absolute pulse energy measurements, the detector setup including absorption in cables and the vacuum window should be characterized with a calibrated THz source. We calculated the pulse energy for different charges (Figure 4) by averaging over all shots during the oscillating autocorrelation measurement. A typical autocorrelation measurement for a charge of 9.4 pC is depicted in Figure 2b. The shape of the autocorrelation is not perfectly symmetric in amplitude and stage position. The amplitude asymmetry could be a result of a nonlinear detector response (onset of saturation). This is in agreement with the slight deviation of the pulse energy from the quadratic fit (Figure 4). Since the length of only one arm is changed and the radiation might not be perfectly collimated, the position scan of the mirror is not creating a perfectly symmetric autocorrelation signal.

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**Author Contributions**

These authors contributed equally to this work. B.H., U.H., P.H., and R.I. conceived the project. U.H. optimized the design. B.H. fabricated the structure and performed the experiments with support from R.I. and A.K. Simulations in CST were performed by G.Y. All authors discussed the results and contributed to the manuscript.

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