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SIMULATION STUDY FOR AN INVERSE DESIGNED NARROWBAND THz RADIATOR FOR ULTRARELATIVISTIC ELECTRONS

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Abstract

THz radiation has many applications, including medical physics, pump-probe experiments, communications, and security systems. Dielectric grating structures can be used to generate cost-effective THz radiation, synchronous to a relativistic beam based on the Smith-Purcell effect. We present a 3D simulation study for the THz radiation emitted from an inverse-designed grating structure after a 3 GeV electron bunch traverses through it. Our farfield simulation results show a narrowband emission spectrum centred around 881 µm, close to the designed value of 900 µm. The grating structure was experimentally tested at the SwissFEL facility, and our simulated spectrum shows good agreement with the observed one.

INTRODUCTION

THz radiation sources are extremely useful in electron acceleration [1–3], wireless communication [4], material and biomedical sciences [5, 6]. The wavelength of this radiation lies between the microwave and infrared regime of the electromagnetic spectrum. Several methods such as optical rectification [7, 8], vacuum tubes and integrated circuits [9, 10] have been used to generate THz radiation. Among these, the Smith-Purcell effect is a cost-effective and compact alternative [11]. Being a precursor of a free electron laser (FEL), this effect is the radiation of light when charged particles pass along periodic metallic or dielectric grating structures. For an electron bunch with relativistic velocity ratio β, the wavelength λ and direction of emitted radiation θ is related to the grating periodicity a by the following Smith-Purcell equation

$$\lambda = \frac{a}{n}\left(\frac{1}{\beta} - \cos\theta\right), \tag{1}$$

where n is the order of the harmonic mode.

Recent advances in computational optimization have paved the way for designing the optical structures algorithmically, purely based on the desired performance and thus skipping the hardships of brute force optimization. Inverse design is such an approach which can be used to devise photonic structures by searching a much broader space of fabricable devices.

Here we present the 3D simulation study of the THz radiation from such a structure designed using the inverse design algorithm [12] and present the comparison with the experimental observation. The structure which we used for investigating the THz radiation was designed using the inverse design method. The optimization process was performed for a single unit cell in a 2D finite-differences frequency-domain simulation (FDFD). Periodic boundary conditions were applied in the direction of electron bunch propagation

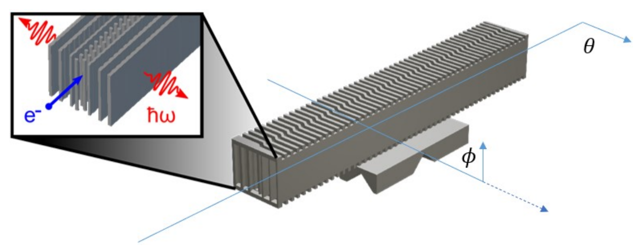

Figure 1: The dielectric grating structure optimized by inverse design approach (top view). Full 3D structure with the base which was experimentally tested in the SwissFEL [13] laboratory and used in 3D time domain simulation. The electron bunch travelled along the grating periodicity direction and the THz radiation was obtained in its perpendicular direction (inset) [14].

and to imitate free space, perfectly matched layers were used. The design was aimed for narrowband THz radiation from ultrarelativistic electrons. In contrast to the conventional metallic gratings for Smith-Purcell radiation, a dielectric structure was used as it has a 1-2 order of magnitude higher damage threshold than metals [15]. The 3D version of the optimized structure is shown in the Fig. 1. The structure was scaled to have a length of 45 mm and a height of 6 mm and fabricated by a 3D printer using stereolithography (SLA) technique. For the dielectric material, Formlabs high tem-

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perature resin was used as it was highly compatible with vacuum after curing at 250°C [16] .

3D TIME DOMAIN SIMULATION

The full 3D time-domain simulations for obtaining the THz radiation spectrum was performed in CST Studio suite [17]. The electron bunch parameters are given in the Table 1.

Table 1: Electron Bunch Parameters

Bunch Parameters	Value
Energy	3 GeV
Transverse width	0.1 mm
Longitudinal width	0.2 mm
Cutoff length	0.4 mm

Due to the extensive computational resource requirement for smaller mesh cell resolutions, the simulation was performed for a longer in time electron bunch than it was used in the experiments. Regardless, this approximation would provide a realistic spectrum for the emitted radiation as the bunch length is still significantly shorter than the targeted central wavelength. Figure 2 shows the simulated time dependent electric field at a probe placed 200 mm far from the grating structures and at $\theta = 90°$ (angle convention from the Fig. 1). The periodic oscillations with multiple frequencies would be the reason of several peaks in the frequency domain (Fourier plane).

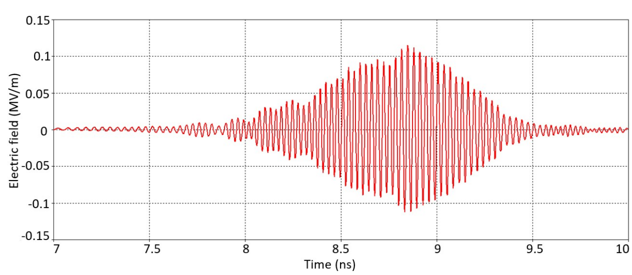

Figure 2: Time-dependent electric field at a far distance (200 mm) from the dielectric structure.

Figure 3 shows the electromagnetic spectrum obtained in CST using its inbuilt farfield monitor at multiple THz frequencies with a wide angular dependence. The radiation is peaked at an angle ≈ 90° and at a frequency of 0.34 THz. Figure 4 shows the strong agreement between the theoretical Smith-Purcell radiation peaks (orange) and the simulated spectrum (blue).

To ensure the usage of sufficient resolution, mesh cell convergence study was performed for the time-domain simulations. This study suggested that a hexahedral type mesh cell having 15 μm of minimum size was enough for accurate results.

COMPARISON OF SIMULATION WITH MEASUREMENT

The grating structure was installed in the ACHIP chamber of the SwissFEL laboratory. A Michelson interferometer

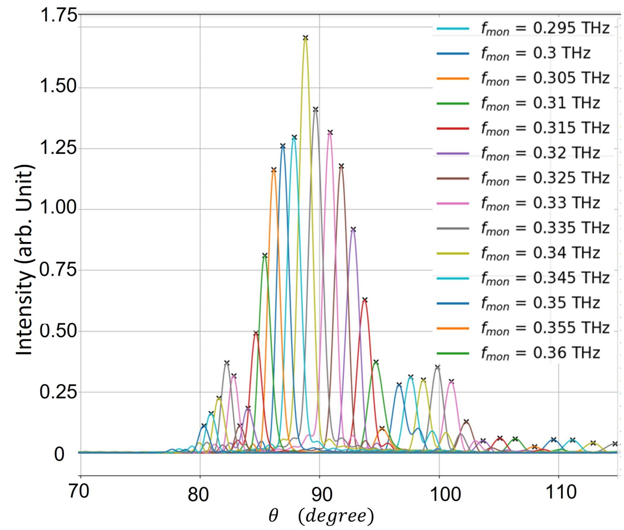

Figure 3: THz radiation spectrum as a function of emission angle obtained by doing a frequency scan at the farfield monitor in CST.

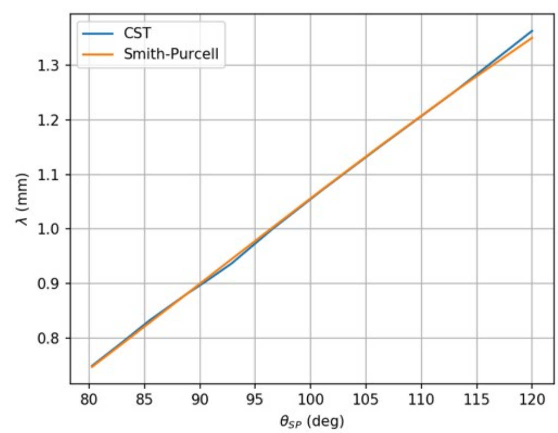

Figure 4: Validation of the THz peaks emitted at different angles from the CST simulation versus the analytical Smith-Purcell equation.

was designed for autocorrelation measurements. A 3.2 GeV electron bunch was sent through the grating structure. The emitted radiation was focused through a lens and then passed through the interferometer before being measured at a detector.

Figure 5 shows the comparison of simulated and the measured electromagnetic spectra. Black curve shows the spectrum measured at SwissFEL laboratory. The green curve is the 3D time-domain simulation in CST and the orange curve is a 3D frequency-domain simulation in COMSOL. The grey color window is the detector's angular acceptance window. The frequency domain spectra is quite narrow compared to the measured one. This is because this simulation considers periodic boundary conditions and the simulation is performed for a single grating period. This suggests that

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the structure theoretically can emit more narrowband radiation, which could be achieved by increasing the number of grating periods. The time domain simulation matches well with the measured spectra and both are approximately peaked at 881 µm. The driving bunch charge was scanned to verify the coherence scaling of energy with the bunch charge.

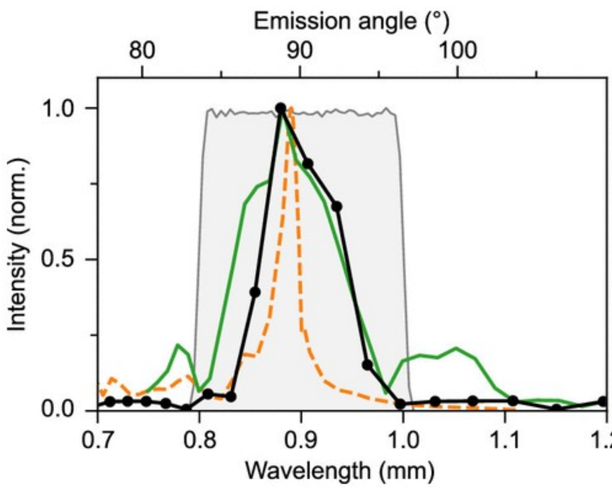

Figure 5: Measured and simulated emission spectrum. Black curve is experimental, orange and green curves are frequency-domain and time-domain simulations [14].

CONCLUSION

We have presented the 3D time-domain simulation study for obtaining THz radiation from an inverse-designed grating structure and presented its comparison with frequency-domain simulations and the measured spectra. The method and the results would have potential applications in future pump-probe experiments and in designing tunable light sources. This kind of design method can provide narrowband and coherent THz radiation at arbitrary wavelengths which would be extremely hard to generate through conventional sources. There is a slight mismatch between the broadness of the time domain spectra and the measured one, and it occurs because of limitations of resolution in both measurements and experiments, which can be surely improved. The structure was fabricated at a resolution of 140 µm, which can be enhanced by present micro/nano lithography techniques. The inverse design was performed for a 2D grating structure and in principle can be developed for 3D optimization. The resolution of the time-domain simulation can be improved by greater computational resources.

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REFERENCES

[1] E. A. Nanni *et al.*, "Terahertz-driven linear electron acceleration," *Nature Communications*, vol. 6, no. 1, pp. 1–8, 2015.

[2] M. T. Hibberd *et al.*, "Acceleration of relativistic beams using laser-generated terahertz pulses," *Nature Photonics*, vol. 14, no. 12, pp. 755–759, 2020.

[3] H. Xu *et al.*, "Cascaded high-gradient terahertz-driven acceleration of relativistic electron beams," *Nature Photonics*, vol. 15, pp. 426–430, 2021.

[4] A. J. Seeds, H. Shams, M. J. Fice, and C. C. Renaud, "Terahertz photonics for wireless communications," *J. Lightwave Technol.*, vol. 33, no. 3, pp. 579–587, 2015.

[5] K. Tanaka, H. Hirori, and M. Nagai, "THz nonlinear spectroscopy of solids," *IEEE Transactions on Terahertz Science and Technology*, vol. 1, no. 1, pp. 301–312, 2011, doi:10.1109/TTHZ.2011.2159535

[6] J.-H. Son, *Terahertz biomedical science and technology*. CRC Press, 2014.

[7] X.-C. Zhang, Y. Jin, and X. F. Ma, "Coherent measurement of THz optical rectification from electro-optic crystals," *Applied Physics Letters*, vol. 61, no. 23, pp. 2764–2766, 1992, doi:10.1063/1.108083

[8] E. A. Schneidmiller, M. V. Yurkov, M. Krasilnikov, and F. Stephan, "Tunable IR/THz source for pump probe experiments at the European XFEL," in *Advances in X-ray Free-Electron Lasers II: Instrumentation*, International Society for Optics and Photonics, vol. 8778, 2013, pp. 151–156, doi:10.1117/12.2017014

[9] J. H. Booske *et al.*, "Vacuum electronic high power terahertz sources," *IEEE Transactions on Terahertz Science and Technology*, vol. 1, no. 1, pp. 54–75, 2011, doi:10.1109/TTHZ.2011.2151610

[10] J. Dai, C. Ruan, Y. Ding, and Z. Yan, "High-power vacuum terahertz photomixer and integrated circuits based on microscale phototubes," *Opt. Express*, vol. 29, no. 2, pp. 1918–1931, 2021, doi:10.1364/OE.409879

[11] S. J. Smith and E. M. Purcell, "Visible light from localized surface charges moving across a grating," *Phys. Rev.*, vol. 92, pp. 1069–1069, 4 1953, doi:10.1103/PhysRev.92.1069

[12] S. Molesky, Z. Lin, A. Y. Piggott, W. Jin, J. Vucković, and A. W. Rodriguez, "Inverse design in nanophotonics," *Nature Photonics*, vol. 12, no. 11, pp. 659–670, 2018.

[13] C. J. Milne *et al.*, "SwissFEL: The Swiss X-ray free electron laser," *Applied Sciences*, vol. 7, no. 7, 2017, doi:10.3390/app7070720

[14] B. Hermann *et al.*, "Inverse-designed narrowband thz radiator for ultrarelativistic electrons," *ACS Photonics*, vol. 9, no. 4, pp. 1143–1149, 2022, doi:10.1021/acsphotonics.1c01932

[15] E. R. Colby, C. McGuinness, K. Soong, R. L. Byer, and E. A. Peralta, "Experimental Determination of Damage Threshold Characteristics of IR Compatible Optical Materials," *Conf. Proc. C*, vol. 110328, pp. 277–279, 2011.

[16] M. Kellermeier *et al.*, "Towards additive manufacturing of dielectric accelerating structures," *Journal of Physics: Conference Series*, vol. 1596, p. 012 020, 2020, doi:10.1088/1742-6596/1596/1/012020

[17] https://www.3ds.com/products-services/simulia/products/cst-studio-suite/,