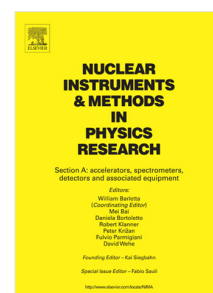


## Accepted Manuscript

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PII: S0168-9002(17)31020-3  
DOI: <https://doi.org/10.1016/j.nima.2017.09.050>  
Reference: NIMA 60129

To appear in: *Nuclear Inst. and Methods in Physics Research, A*

Received date: 28 December 2016

Revised date: 24 July 2017

Accepted date: 20 September 2017

Please cite this article as: Y. Wei, R. Ischebeck, M. Dehler, E. Ferrari, N. Hiller, S. Jamison, G. Xia, K. Hanahoe, Y. Li, J.D.A. Smith, C.P. Welsch, Investigations into dual-grating THz-driven accelerators, *Nuclear Inst. and Methods in Physics Research, A* (2017), <https://doi.org/10.1016/j.nima.2017.09.050>

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## Investigations into dual-grating THz-driven accelerators

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### Abstract

Advanced acceleration technologies are receiving considerable interest in order to miniaturize future particle accelerators. One such technology is the dual-grating dielectric structures, which can support accelerating fields one to two orders of magnitude higher than the metal RF cavities in conventional accelerators. This opens up the possibility of enabling high accelerating gradients of up to several GV/m. This paper investigates numerically a quartz dual-grating structure which is driven by THz pulses to accelerate electrons. Geometry optimizations are carried out to achieve the trade-offs between accelerating gradient and vacuum channel gap. A realistic electron bunch available from the future Compact Linear Accelerator for Research and Applications (CLARA) is loaded into an optimized 100-period dual-grating structure for a detailed wakefield study. A THz pulse is then employed to interact with this CLARA bunch in the optimized structure. The computed beam quality is analyzed in terms of emittance, energy spread and loaded accelerating gradient. The simulations show that an accelerating gradient of  $348 \pm 12$  MV/m with an emittance growth of 3.0% can be obtained.

**Keywords:** Dielectric dual-gratings, THz-driven, high gradient, wakefield, THz-bunch interaction, beam quality

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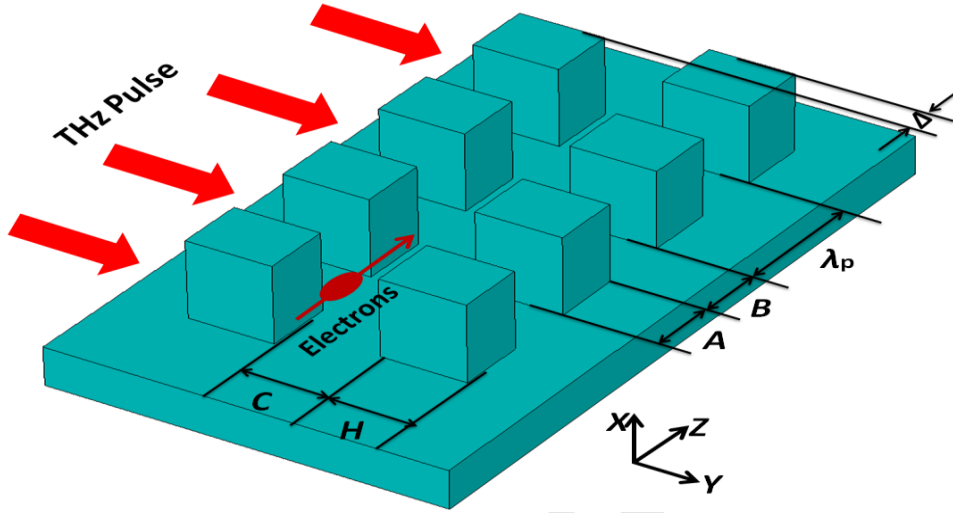
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**26 1. Introduction**

27 Dielectric structures have been found to withstand electric fields one to two orders of magnitude larger than  
28 metals at optical frequencies, thereby sustaining high accelerating gradients in the range of GV/m. These  
29 dielectric structures can be driven either by infrared optical or by THz pulses, enabling dielectric laser-driven  
30 accelerators (DLAs) and dielectric THz-driven accelerators (DTAs). Empirically, it is found that the RF-induced  
31 breakdown threshold  $E_s$  scales with frequency as  $f^{1/2}$  and pulse duration as  $\tau^{-1/4}$ , as described in  $E_s \propto f^{1/2}\tau^{-1/4}$   
32 [1,2]. This indicates that in principle, DLAs can generate accelerating gradients higher than DTAs. DLAs have  
33 successfully demonstrated accelerating gradients of 300 MV/m [3] and 690 MV/m [4] for relativistic electron  
34 acceleration, and gradients of 25 MV/m [5], 220 MV/m [6] and 370 MV/m [7] for non-relativistic electron  
35 acceleration. However, DLAs suffer from low bunch charge and sub-femtosecond timing requirements due to the  
36 short wavelength of operation. In a DLA, a laser beam is used to accelerate particles through a microscopic  
37 channel in an artfully-crafted glass chip. Such a channel gap can be no wider than several  $\mu\text{m}$  [3,4,8-12] in order  
38 to generate a high gradient of GV/m, which limits the transverse size and hence the bunch charge. Furthermore,  
39 for a laser wavelength of 2  $\mu\text{m}$ , the particle bunch has to occupy only a small fraction of the optical cycle in order  
40 to maintain good beam quality in terms of emittance and energy spread. If  $1^0$  of optical cycle is used, the total  
41 bunch length is only 5.6 nm, which also limits the particle bunch charge. In addition, the timing precision  
42 between the optical cycle and the arrival of the particle bunch is a practical concern. Using a laser wavelength of  
43 2  $\mu\text{m}$ , a  $1^0$  phase jitter requires a timing jitter of  $< 20$  as between the optical pulse and the particle bunch, which is  
44 challenging to maintain over long distances.

45 THz frequencies provide wavelengths two orders of magnitude longer than optical sources. In this situation,  
46 DTAs can be fabricated with conventional machining techniques due to the long wavelength of operation. This  
47 accommodates particle bunches with larger sizes and charges, which is more beneficial for bending and focusing  
48 [13] compared to DLAs. DTAs also provide a more accurate timing jitter than DLAs. For a THz wavelength of  
49  $600\ \mu\text{m}$ ,  $1^\circ$  of optical cycle corresponds to a  $1.7\ \mu\text{m}$  bunch length, while  $1^\circ$  of phase jitter requires a  $5.6\ \text{fs}$  timing  
50 jitter, which is readily achievable [14]. With recent advances in sources for the generation of THz, mJ pulse  
51 energy and extremely high electric fields in the GV/m have been achieved [15-17], which can boost the  
52 accelerating gradient up to GV/m for a DTA. Experiments have already demonstrated the acceleration of  
53 electrons in THz-driven dielectric structures [18-20]. Therefore, DTAs are holding great potential for reducing  
54 the size and cost of future particle accelerators.

55 In this paper a quartz dual-grating structure is investigated for accelerating electrons at THz frequencies. As  
56 shown schematically in Fig. 1, a short, intense THz pulse is used to illuminate a dual-grating structure, creating  
57 standing-wave-like electric field in the structure's channel gap where the electrons travel and are accelerated. In  
58 Section 2, geometry optimizations are performed in order to find the optimum dual-grating structure for the  
59 acceleration of relativistic electrons. It is then followed in Section 3 by a detailed wakefield study of an optimized  
60 100-period dual-grating structure. Simulations are performed using the beam properties of the future Compact  
61 Linear Accelerator for Research and Applications (CLARA) [21] which is planned as an X-ray free electron laser  
62 (FEL) test facility located at the Daresbury laboratory in the UK. In Section 4, a linearly-polarized THz pulse is  
63 introduced to interact with the CLARA bunch in the optimized structure. The achievable beam quality is analyzed  
64 in terms of emittance, energy spread and loaded accelerating gradient. Finally the current challenges and  
65 limitations are discussed.



66  
 67 Fig. 1. Schematic of a dual-grating structure illuminated by a THz pulse.  $\lambda_p$ ,  $A$ ,  $B$ ,  $C$ ,  $H$ , and  $\Delta$  represent grating period, pillar  
 68 width, pillar trench, vacuum channel gap, pillar height and longitudinal shift, respectively;  $A + B = \lambda_p$  is selected for all  
 69 simulations.

## 70 2. Geometry optimization

71 The dual-grating structure is a modification from the original design by Plettner *et al.* [8]. When a linearly-  
 72 polarized THz pulse travels through the structure, the speed of the wave in vacuum is higher than that in the  
 73 dielectric grating pillar. This produces the desired  $\pi$  phase difference in the vacuum channel for the wave front,  
 74 resulting in periodic energy modulation for electrons travelling along the longitudinal  $z$ -axis.

75 In order to optimize such a dual-grating structure, VSim [22], based on a finite difference time domain  
 76 (FDTD) method, is used to compute the electric and magnetic fields generated in the structure. The gratings are  
 77 modelled as a 2-dimensional ( $y$ - $z$  plane) structure to simplify our computations for the electric and magnetic  
 78 fields. Periodic boundary conditions are applied along the electron channel in the  $z$  direction. Matched absorbing  
 79 layers (MALs) are used along the laser propagation direction ( $y$ -axis) to absorb the transmitted wave. The mesh  
 80 size is set to  $\lambda_p/80$  so that the simulation results are converged to increase accuracy

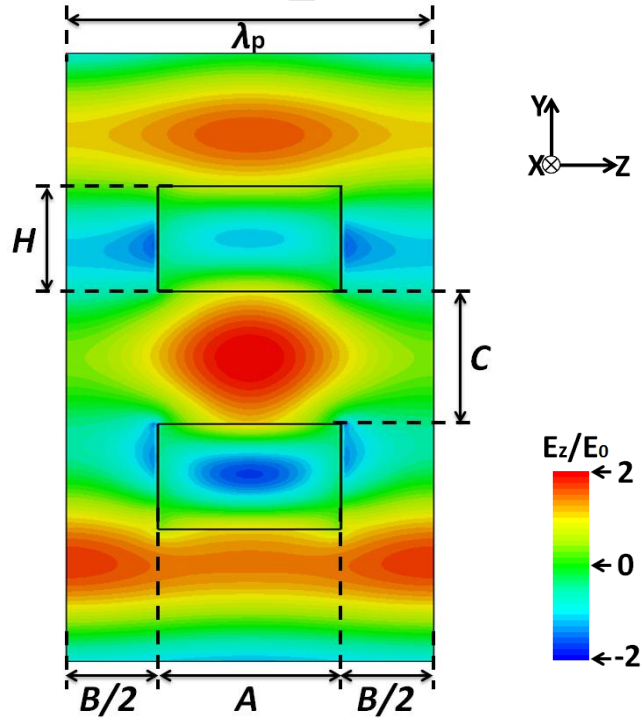
81 A plane wave with a wavelength of  $\lambda_0 = 150 \mu\text{m}$  and a field amplitude  $E_0$  propagates in  $+y$  and illuminates a  
 82 single unit dual-grating structure, as illustrated in Fig. 2. A grating period of  $\lambda_p = 150 \mu\text{m}$  is chosen so that the  
 83 first spatial harmonic and relativistic electrons are synchronized [23]. The desired  $\pi$  phase difference for the wave

84 front is achieved by setting pillar height  $H = \frac{\lambda_0}{2(n-1)} = 0.50\lambda_0$ , here quartz with a refractive index of  $n = 2$  [Ref. 24]  
 85 is chosen due to its high damage threshold [18-20,25-27] and thermal conductivity.

86 The accelerating gradient  $G_0$  is evaluated by  $E_z[z(t), t]$  which is the longitudinal electric field integral along  
 87 the vacuum channel center as shown in Fig. 2:

$$88 \quad G_0 = \frac{1}{\lambda_p} \int_0^{\lambda_p} E_z[z(t), t] dz, \quad (1)$$

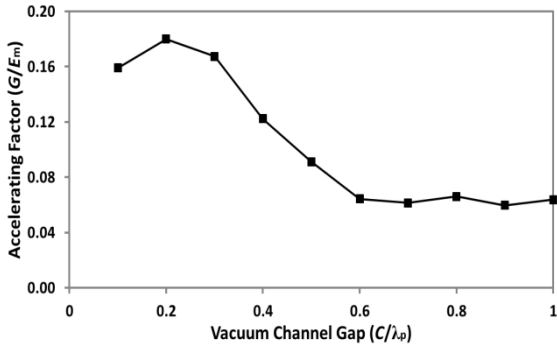
89 where  $\lambda_p$  is the grating period,  $z(t)$  is the position of the electrons in the vacuum channel at time  $t$ . To find the  
 90 maximum accelerating gradient, we need to maximize the electric field distributed in the structure, which should  
 91 not exceed the material damage field. So an accelerating factor [28] ( $AF = G_0/E_m$ ) is defined by the ratio of the  
 92 accelerating gradient  $G_0$  to the maximum electric field  $E_m$  in the structure.



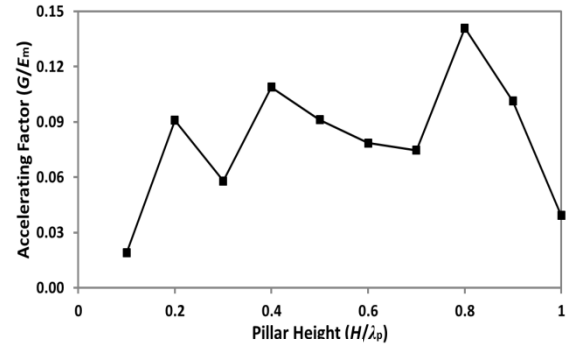
93  
 94 Fig. 2. Longitudinal electric field  $E_z$  distribution in a single unit dual-grating structure illuminated by a uniform plane wave  
 95 with a field  $E_0$  along  $y$ -axis.

96 A detailed geometry optimization is carried out to maximize the accelerating factor  $AF$  with the widest  
 97 channel gap  $C$ . For an initial pillar height  $H = 0.50\lambda_0$ , a maximum accelerating factor  $AF = 0.18$  can be achieved

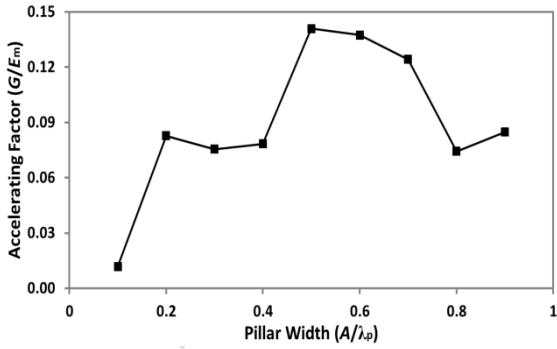
108 when the vacuum channel gap  $C = 0.20\lambda_0$  as seen in Fig. 3(a). When  $C$  increases from  $0.20\lambda_0$ , the accelerating  
 109 factor  $AF$  gradually decreases, which can be seen in Fig. 3(a). This means that the achievable gradient gradually  
 100 drops with  $C > 0.2\lambda_0$ , so a channel gap of  $C = 0.50\lambda_p$  is chosen as an acceptable parameter due to a trade-off  
 101 between the accelerating gradient and available phase space in which high accelerating gradient occurs. As  
 102 shown in Fig. 3(b), a maximum accelerating factor ( $AF = 0.141$ ) appears at a pillar height of  $H = 0.80\lambda_p$  for the  
 103 structure with an optimum channel gap,  $C = 0.50\lambda_p$ . Fixing the grating structure,  $C = 0.50\lambda_p$  and  $H = 0.80\lambda_p$ , we  
 104 then set out to find the optimal pillar width  $A$ . Figure 3(c) shows  $AF = 0.141$  can be obtained for a pillar width  $A$   
 105  $= 0.50\lambda_p$ . The longitudinal shift  $\Delta$  between the gratings is also investigated. It can be seen from Fig. 3(d) that the  
 106 maximum  $AF = 0.141$  occurs when perfectly aligned ( $\Delta = 0$  m). However, the worst shift can reduce the  
 107 accelerating factor by a factor of 54% to  $AF = 0.065$ . The damage threshold for quartz at THz frequencies is  
 108 found experimentally to be  $\sim 13.8$  GV/m [25]. So a maximum accelerating factor of  $AF = 0.141$  corresponds to a  
 109 maximum achievable gradient of  $0.141 \times 13.8 = 1.95$  GV/m for a quartz dual-grating structure.



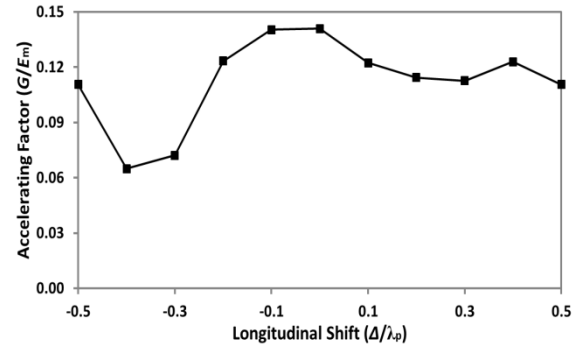
(a)



(b)



(c)



(d)

123

124 Fig. 3. FDTD optimization of accelerating factor  $AF$  as a function of (a) vacuum channel gap  $C$  with a fixed pillar height  $H =$   
 125  $0.50\lambda_p$ , (b)  $H$  with a fixed  $C = 0.50\lambda_p$ , (c) pillar width  $A$  with a fixed  $C = 0.50\lambda_p$  and  $H = 0.80\lambda_p$ , and (d) longitudinal shift  $\Delta$   
 126 with a fixed  $C = 0.50\lambda_p$ ,  $H = 0.80\lambda_p$  and  $A = 0.50\lambda_p$ .

### 127 3. Wakefield study for the optimized structure

128 After geometry optimization, a dual-grating structure with a channel gap of  $C = 0.50\lambda_p$ , pillar height of  $H =$   
 129  $0.80\lambda_p$ , pillar width of  $A = 0.50\lambda_p$ , longitudinal shift of  $\Delta = 0$  m and grating period of  $\lambda_p = 150$   $\mu\text{m}$  is desirable as  
 130 an optimum choice for the following study. In this section, detailed wakefield study are carried out by loading an  
 131 electron bunch from future CLARA into such an optimized 100-period dual-grating structure without THz  
 132 illumination.

133 The bunch parameters from future CLARA are listed in Table 1. When CLARA works at ultra-short pulse  
 134 mode [21], a short electron bunch with a longitudinal RMS length of 90  $\mu\text{m}$  can be generated. Assuming 10% of  
 135 the initial charge of 3 pC is transmitted through the energy collimators, so an electron bunch with a charge of 0.3  
 136 pC can be obtained. Then it can be focused by a permanent magnetic quadrupole to give a transverse RMS radius  
 137 of 5  $\mu\text{m}$ , as shown in Table 1.

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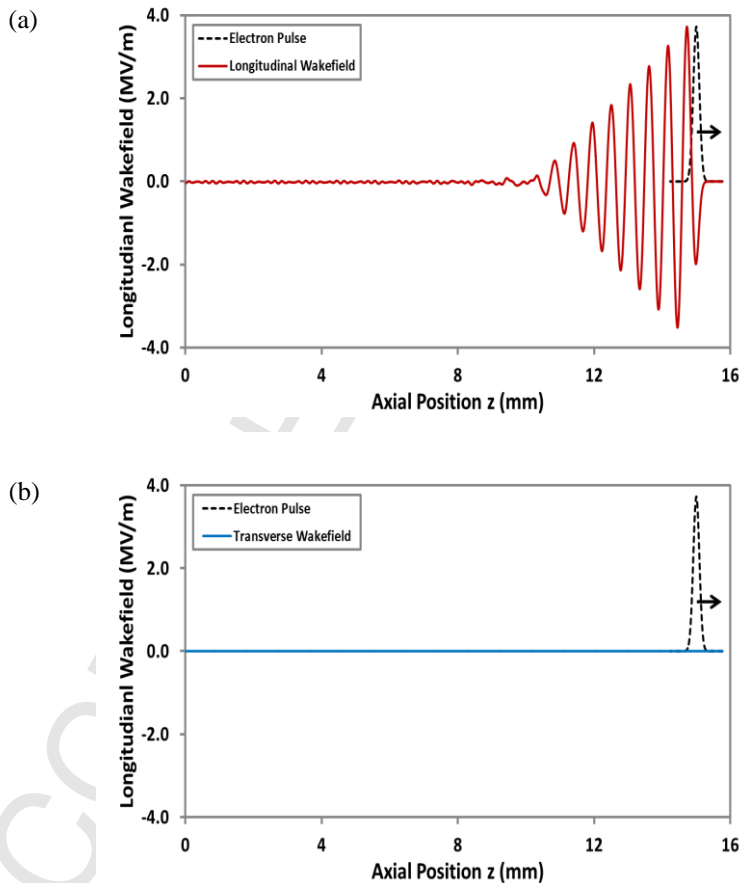
Table 1. CLARA bunch parameters used in the simulation

Bunch parameters	CLARA	Simulation
Bunch energy [MeV]	50	50
Bunch charge [pC]	$\leq 250$	0.3
Bunch RMS length [ $\mu\text{m}$ ]	9-300	90
Bunch RMS radius [ $\mu\text{m}$ ]	10-100	5
Normalized emittance [mm·mrad]	$\leq 1$	0.15
Energy spread	$< 0.1\%$	0.05%

139 When such an electron bunch with Gaussian profiles is injected to travel along the channel centre of the  
 140 optimized structure without any offset in the  $y$  direction, it generates electromagnetic fields that propagate in the  
 141 vacuum channel. The wakefields are reflected back by dielectric gratings and interact with the bunch itself, thus  
 142 resulting in energy loss or deflection for electrons in the bunch. Here, the Wakefield Solver of CST [29] is used to  
 143 calculate the wakefield generated in the optimized structure. It is then followed by a VSim Particle-In-Cell (PIC)  
 144 simulation which is performed to analyze the effect of wakefield for the bunch in terms of emittance and energy



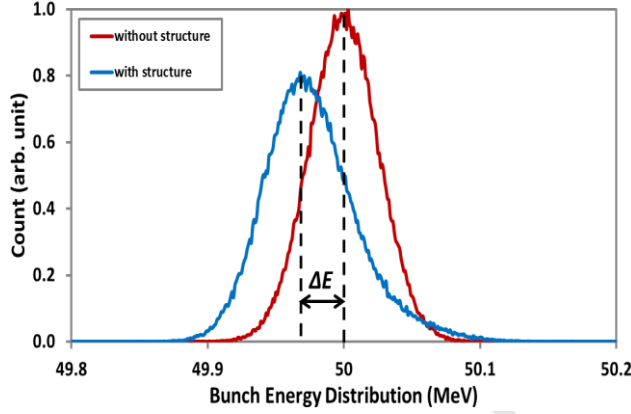
145 spread. The longitudinal ( $z$ -component) and transverse ( $y$ -component) wakefield distribution on  $z$ -axis in the  
 146 structure are illustrated in Fig. 4. Fig. 4(a) gives a maximum longitudinal decelerating wakefield of 2.00 MV/m  
 147 for the bunch. It agrees well with the final bunch energy distribution as given in Fig. 5 which gives an energy  
 148 spread of 0.068% and average energy loss of  $\Delta E = 30.0 \pm 1.0$  keV for the whole bunch, corresponding to a  
 149 decelerating field of  $2.00 \pm 0.07$  MV/m. In addition, the transverse wakefield, which deflects electrons, is  
 150 negligible as given in Fig. 4(b) due to a small transverse size and symmetrical Gaussian profile in the  $y$  direction.  
 151 This is in accordance with results from particle tracking simulations showing that when the bunch travels out of  
 152 the structure, the normalized RMS emittance is still  $0.15 \mu\text{m}$ , remaining the same as that of initial time.



153

154

155 Fig. 4. Simulated longitudinal (a) and transverse (b) wakefield distribution on  $z$ -axis. The electron bunch travels along the  $z$ -  
 156 axis.



157

158 Fig. 5. The bunch energy distribution without structure (red line) shows an energy spread  $\sim 25$  keV (0.05%) whereas the  
 159 bunch going through the structure (blue line) shows an energy spread  $\sim 34$  keV (0.068%).

#### 160 4. THz-Bunch interaction in the optimized structure

161 In this section, a linearly polarized Gaussian THz pulse, as shown in Fig. 6, is launched to propagate along  
 162 the  $y$ -axis in order to interact with the CLARA bunch in the vacuum channel centre of the optimized structure.  
 163 All relevant parameters are described in Table 2. Here, the peak field of THz pulse is set to 1.0 GV/m, which can  
 164 be obtained from a multi-cycle THz pulse with mJ energy proposed by *K. Ravi et al.* [30]. This field is still below  
 165 the quartz damage threshold. In its co-moving frame, the bunch experiences the strongest field in the channel  
 166 centre through precise timing calculation. Considering Gaussian temporal and spatial distributions, the electrons

167 experience a temporal electric field  $E_t = G_p e^{-\left(\frac{z}{w_{\text{int}}}\right)^2}$  [Ref. 31] with a characteristic interaction length  $w_{\text{int}} =$

168  $\left(\frac{1}{w_z^2} + \frac{2\ln 2}{(\beta c \tau_p)^2}\right)^{-0.5} = 454 \mu\text{m}$ . When a peak accelerating gradient of  $G_p = 1.0$  GV/m is assumed for integration of

169 this field  $E_t$ , a maximum energy gain of  $\Delta E_m \approx 805$  keV is generated, which can be used to calculate the  
 170 accelerating gradient for the following simulations.

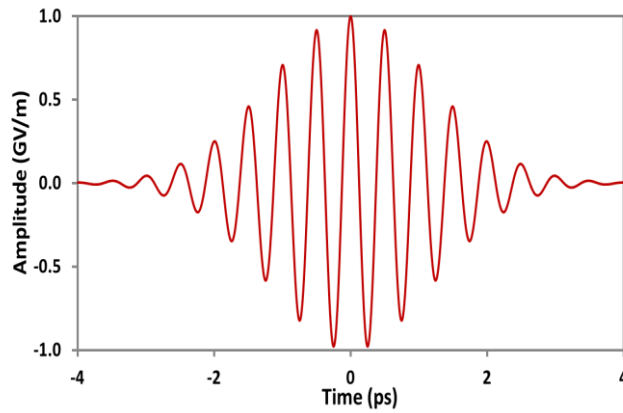


Fig. 6. The electric field envelope of the THz pulse.

Table 2. Parameters of the THz pulse used in the simulation.

THz pulse characteristics	
Propagation direction	+ y
Wavelength $\lambda$	150 $\mu\text{m}$
Frequency $f$	2.0 THz
Peak field	1.0 GV/m
FWHM duration $\tau$	2 ps
Waist radius $w_z$	1.0 mm

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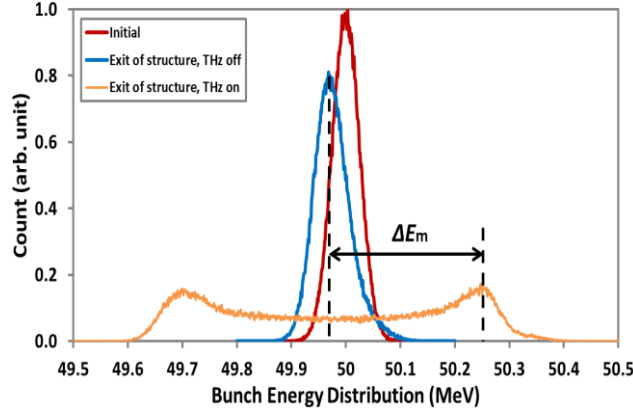
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A PIC simulation is then carried out using the same bunch parameters from future CLARA, so the electrons will experience a field superposition of the particle's wakefields and the driving field produced from the THz pulse. From particle tracking results, it is found that the transverse RMS emittance is 0.155  $\mu\text{m}$  when the bunch travels out of the structure, corresponding to an increase of 3.0% compared to that of the THz-off case. This minor increment can be explained by a weak deflecting force excited by the THz pulse. However, this deflecting force does not change the bunch transverse emittance significantly at such short interaction distance. In addition, it can be compensated by a symmetric illumination using two THz pulses from opposite sides.



182

183 Fig. 7. The energy distribution for the initial bunch (red line), and the bunch exiting of the optimized structure when THz is  
 184 off (blue line) and on (yellow line).

185 The electron bunch has an RMS length of  $\sigma_z = 90 \mu\text{m}$ , so most electrons in the range of  $\pm \sigma_z$  are able to  
 186 sample all phases of the THz field. Each slice of electrons ( $\Delta t \ll \lambda_0/c$ ) samples a different phase of sinusoidal  
 187 electric field in the vacuum channel and thereby experience a corresponding net energy shift  $g(\Delta t, \Delta E_m) =$   
 188  $\Delta E_m \cos\left(\frac{2\pi c}{\lambda_0} \Delta t\right)$ , where  $\Delta E_m$  is the maximum energy gain for the electrons. This will cause some electrons to  
 189 gain energy from acceleration while others are decelerated, which generates a double-peaked profile for final  
 190 bunch energy distribution, as shown in Fig. 7. The final bunch has an energy spread of 0.42% when calculated  
 191 with particle tracking simulations. It is also found that the maximum energy gain is  $\Delta E_m = 280 \pm 10 \text{ keV}$ ,  
 192 corresponding to a maximum accelerating gradient of  $G_m = 348 \pm 12 \text{ MV/m}$ . Here when the peak field of a THz  
 193 pulse is increased to  $E_p = 3.0 \text{ GV/m}$ , an accelerating gradient greater than 1.0 GV/m can be expected for such a  
 194 structure. It can be seen from the simulation that such a THz field of 3.0 GV/m leads to a maximum field of 9.37  
 195 GV/m, which is still below the damage threshold for quartz structures.

## 196 5. Summary and outlook

197 This paper presents numerical simulations for a THz-driven dual-grating structure to accelerate electrons  
 198 including geometry optimizations, wakefield and THz-bunch interaction study in detail. Geometry studies have  
 199 been carried out to maximize the accelerating factor with the widest channel gap  $C$ . For an optimized structure

200 with a channel gap of  $C = 0.50\lambda_p$ , pillar height of  $H = 0.80\lambda_p$ , pillar width of  $A=0.50\lambda_p$  and longitudinal shift of  $\Delta$   
201  $= 0$  m, a maximum accelerating factor  $AF = 0.141$  can be obtained, corresponding to a maximum unloaded  
202 gradient of  $G = 1.95$  GV/m. Using CST and VSim, a Gaussian electron bunch from future CLARA is loaded into  
203 an optimized 100-period structure for detailed wakefield study. When the bunch travels out of the optimized  
204 structure, the average energy is reduced by  $30.0 \pm 1.0$  keV due to its interaction with longitudinal decelerating  
205 wakefield. The transverse wakefield can be negligible so that it does not have any effect on the bunch emittance.  
206 Then an intense THz pulse is added into simulation to interact with the CLARA bunch in the optimized structure.  
207 When the bunch propagates out of the structure, the transverse RMS emittance increases by 3.0% compared to  
208 that of THz-off case, the energy spread changes from 0.05% to 0.42%, and an accelerating gradient of  $348 \pm 12$   
209 MV/m could be expected from the particle tracking simulations.

210 These simulations have demonstrated numerically the high gradient acceleration of electrons in a dual-  
211 grating structure driven by THz pulses, with a small emittance increase. However, there are still some technical  
212 challenges to implementing it in reality. Firstly, despite some experiments which have generated multi-cycle THz  
213 pulses with nJ [32] and  $\mu$ J energies [33], further development is needed to obtain THz pulses with mJ energies, to  
214 generate the peak field of 1 GV/m which is assumed for our simulations. The second challenge is to improve the  
215 electrons' energy gain, which is limited by the short THz-bunch interaction length caused by the wide band-  
216 widths of excitation and structures. A principal option for DLAs would be to tilt the front of the laser pulses by  
217 diffraction gratings to extend the interaction length, thereby increasing the electrons' energy gain. However, THz  
218 pulses cannot be operated in a similar way due to their wide bandwidth [34]. Instead, for DTAs a multilayer  
219 dielectric Bragg reflector [12] could be incorporated into the structure to boost the accelerating field in the  
220 channel, which has the potential to increase the energy gain. Further research efforts on fabrication and  
221 experiments are still required to pave the way for a realistic high-energy DTA concept.

222

223 **Acknowledgements**

224 We would like to thank Dr. Mark Ibison for carefully proof-reading the original manuscript. This work is  
 225 supported by the EU under Grant Agreement 289191 and the STFC Cockcroft Institute core grant  
 226 No.ST/G008248/1.

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