Design strategies for single-cycle ultrafast electron guns

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Abstract

After the first introduction of ultrafast electron guns for acceleration of particles using single-cycle electro-magnetic pulses, the basic structure has gained increasing interest as promising solutions for high gradient compact electron guns. The significant benefit of using transient ultrashort pulses in this acceleration scheme opens a realistic path towards gigavolt-per-meter acceleration gradients. In this paper, we present an optimized design strategy for these electron guns. The goal is to estimate the THz energy needed for an optimum device to accelerate electrons at rest to a certain energy using materials that endure a pre-determined maximum electric field. We start with designing a gun delivering 400 keV electron beam energy and discuss different techniques to enhance the performance. Throughout this design process, it is implicitly shown that the concept of single-cycle ultrafast electron guns can apply THz beams with energies in the level of 100–400 μJ to accelerate electrons, which is the state-of-the-art technology in THz radiation sources. Subsequently, upgrading the design to an 800 keV device is outlined, to demonstrate the eligibility of this concept to perform as linac injectors in compact accelerator facilities.

Keywords: accelerator physics, electron gun, THz acceleration, transient pulses, ultrafast physics

(Some figures may appear in colour only in the online journal)

1. Introduction

The past century has witnessed the major role played by particle accelerators in achieving breakthrough discoveries in fundamental research using advanced instruments like high-energy colliders [1, 2], x-ray light sources [3–6], and electron diffractometers [7–10]. The first and most critical stage of an accelerator facility is the gun, which accelerates particles initially at rest to relativistic speeds. Therefore, many limitations in accelerator operation and particle beam quality are set by the gun properties. For example, the intense Coulomb repulsion of particles at low energies results in emittance growth of the electron beam. The conservation of emittance in the relativistic regime subsequently transfers this degrading effect to the ultimate operation point of the user facility. As a consequence, electron guns with high acceleration gradients are always sought after to produce relativistic particles in the shortest possible time and distance, thereby preventing the emittance growth of the injected bunch [11–14].

The conventional electron gun technology is based on either high DC voltages or RF radiation. DC guns suffer from severe limitations in acceleration gradient and the final acceleration energy, making it very challenging to produce more than 0.5 MeV electron beams [15]. RF guns, as promising suppliants for DC devices, have achieved optimum performance for accelerating large bunches of about ~1 nC size [16]. However, they are neither energy nor cost efficient when acceleration of 1–10 pC-level bunches is pursued. Some other difficulties in the construction of such guns are the bulky and expensive high voltage feedthroughs for DC guns, and high power klystrons needed to power RF guns. In
addition, synchronization challenges between RF guns and lasers hinder the progress to achieve short electron bunches and smaller devices. The need for more economical devices, in conjunction with the desire for higher field strengths, has propelled extensive research efforts towards realization of novel accelerators with higher field breakdown thresholds and intrinsic synchronization.

Investigating damage mechanisms in accelerators is of key importance to invent new approaches for boosting the achievable acceleration gradient. The empirical studies done by Loew and Wang had initially shown that electron field emission, scaling as $f^{0.5} \tau^{-0.25}$ with $f$ the operation frequency, and $\tau$ the pulse duration of the accelerating field, imposes a principal limit on device performance [17]. However, recent comprehensive studies on breakdown thresholds of various accelerators demonstrated that pulsed heating of the accelerator walls is the dominant factor limiting acceleration gradients [18, 19]. This conclusion confirmed the observed lower operational gradients in existing facilities when compared with predictions from the previously derived scaling laws. The authors concluded that the pulse duration of the accelerating field plays the major role in the breakdown event, since it is directly linked to the pulse energy governing pulsed heating in the device. In parallel, the recent detailed studies of breakdown rates in RF accelerators have confirmed this conclusion [20]. The principal outcome of these studies was the value of $E_{\text{max}}^6 \tau$ being constant in various facilities operating based on micro-second long pulses in RF regime. Therefore, venues for obtaining higher acceleration gradients can be found in short pulse regimes. For example, using picosecond long pulses will augment the possible acceleration gradients by at least a factor of ten, making 0.5 GV m$^{-1}$ a safe assumption for accelerator design.

Based on the above investigations, one can think of three approaches for pushing the limits of acceleration gradient. First, one may try to realize accelerating fields without any surrounding materials or boundaries. Such an approach results in the creative field of laser-plasma wakefield acceleration, where electrons are accelerated in the wakefields of a plasma [21–30] with THz frequencies. Second, increasing the operation frequency is a proper path from different viewpoints. Higher operation frequency shrinks down the device dimensions, which in turn reduces the required energy for particle acceleration. This relaxes limitations due to pulsed heating. Furthermore, higher field emission thresholds as well as easier realization of short pulses assist in obtaining high gradient accelerators. Dielectric laser accelerators [31–33] and THz-driven linear electron acceleration [34, 35] are promising outcomes of this approach. A promising solution that we have introduced is the concept of single-cycle ultrafast electron guns, which are accelerators excited by single-cycle pulses [36]. The ultrashort time over which the device boundaries are affected by high fields enables the possibility of achieving high acceleration gradients in these new accelerators. The experimental efforts towards implementation of these devices have shown their feasibility and promise for both acceleration and electron beam manipulation [37–40]. The concept of the device is thoroughly introduced and discussed in [36]. In this paper, we present the detailed procedure how an optimum electron gun is designed.

A complete definition of the design problem is described in the next section. We start with the description of the single-cycle ultrafast gun concept and proceed with the problem definition. Subsequently, the design process is presented as main part of this paper in section 3. Section 4 discusses techniques for fine tuning the design to enhance the output bunch characteristics. The next section presents the outcome of the presented process used for designing an ultrafast electron gun with higher electron beam energy than the first design. Finally, section 6 concludes the paper.

2. Problem definition

2.1. Single-cycle ultrafast gun concept

Figure 1 schematically illustrates a single-cycle ultrafast electron gun, which consists of three principal sections, interaction region, focusing section, and coupler. It is assumed that two linearly polarized single-cycle Gaussian beams symmetrically impinge on the device from both sides. The coupler section transfers the energy of the Gaussian beam into the multilayer focusing section, where two metallic walls on both sides focus the beam into the interaction region. The
accelerating cycle of the demonstrates continuous interaction of particles with the ultrafast electron guns is visualized in with traveling electrons. The acceleration process in these substantiates phase-front matching of the incoming pulses accelerating cycle of the pulse. In other words, the device assures continuous interaction of traveling electrons with the interaction region in each layer can be considered as a rectangular waveguide, whose TE_{01} mode is excited by the incoming fields from the focusing section. At the interaction region, the transverse and longitudinal magnetic fields of the two counter-propagating TE_{01} modes cancel each other, whereas the vertical electric field will be constructively added. The superposition of these two beams results in a purely accelerating field along the z-axis in figure 1.

Starting in the coupler section, horizontal metallic plates, called here separators, divide the incoming Gaussian beam into several regions with thickness $d_j$. The energy in each region is then guided to each sub-waveguide of the gun. The traveling pulse entering each focusing section is subsequently delayed by dielectric inclusions, whose lengths $L_j$, are designed to control the arrival of pulses into the interaction region. Proper design of the two sets of parameters $d_j$ and $L_j$ assures continuous interaction of traveling electrons with accelerating cycle of the pulse. In other words, the device substantiates phase-front matching of the incoming pulses with traveling electrons. The acceleration process in these ultrafast electron guns is visualized in figure 2. Snapshots of field profiles are superposed on particle profiles, which demonstrates continuous interaction of particles with the accelerating cycle of the field.

Various significant improvements are considered compared with the geometries presented in [36]. Previously, the dielectric contrast in each layer was realized by the two materials Teflon and Quartz. The requirements for mechanical stability of the thin separators necessitated filling the focusing sections with rigid materials. However, as will be observed in the fine tuning section, thick separators are advantageous for reducing the energy spread of the output bunch. Once thick metallic plates are used to divide the input energy among different sections, the need for filled focusing spaces is remedied. Therefore, one can rely on the dielectric contrast between vacuum and quartz to reach the goal with respect to phase-front matching. The second change is the open slot in the interaction region devised for incoupling of the photoinjector laser. The old configuration accounted for a back-illuminated photocathode structure [36]. Nonetheless, our recent experimental investigations revealed some difficulties in extracting large amount of charge from thin metallic coatings in such type of cathodes [38]. The open narrow slot in the interaction region enables electron output as well as easy input coupling of the photoinjector laser from the front side, without dramatically disturbing the accelerating field profile. Furthermore, the coupler section in figure 1 takes flat separators into account. This differs with the structure shown in [36], where minute inclinations are considered to gain a uniform acceleration gradient over the layers. Since a constant acceleration gradient is not a crucial requirement for the operation of these devices, the burden caused by these oblique separators in the fabrication process can simply be avoided through the assumption of flat separators.

2.2. Design problem

Based on the above concept, ultrafast electron guns with unprecedented high accelerating fields can be implemented. For this purpose, a design process needs to be followed to achieve optimal operation. In other words, a design problem should be defined and systematically solved. Let us suppose that the gun is made out of a material that supports stable operation with maximum electric field $E_{\text{max}}$ in the single-cycle operation regime. The desire to achieve high acceleration gradients and high quality bunches often inspires operation of accelerating devices close to damage threshold. The largest surface field in the proposed device exists over the photocathode surface, where the two incoming pulses interfere constructively in the proximity of a metallic surface. In the next layers, the above interference effect occurs in the vacuum region. Hence, the maximum acceleration gradient is equal to the maximum normal field strength, i.e. $E_{\text{max}}$. On the other hand, as observed in figure 1, the superposition of two fields with opposite signs at the separators considerably reduces the field strengths around the edges in the gun geometry. Consequently, despite the field enhancement due to the edge effects, the field strengths at these regions do not exceed the photocathode surface field. The design problem consequently aims at a device which realizes peak accelerating fields equal to $E_{\text{max}}$, using a minimum required energy in the two incoming Gaussian beams.

Figure 2. Illustration of the phase-front matching of the single-cycle pulse with the accelerating electron bunch: (a)–(f) snapshots of the field profile and bunch distribution when the bunch center resides in the first five layer.
3. Design process

To explain how such an optimum design can be achieved, we take an exemplary problem into account. We aim to design a 400 keV electron gun fed by single-cycle THz pulses centered at 300 GHz with a copper photocathode. From the previous investigations and scaling laws, the value of $E_{\text{max}}$ is assumed to be around 600 MV m$^{-1}$ [38]. Once the acceleration gradient and operation frequency is fixed to 600 MV m$^{-1}$ and 300 GHz, the interaction section, shown and parameterized in figure 3(a), is designed using an analytical formulation.

To determine the transverse sizes of the interaction section, $d_e$ and $d_s$, the accelerating field profile of the two counter-propagating TE01 modes needs to be considered, which reads as

$$E_z = A \cos \pi \left( e^{-i k_s x} + e^{-i k_s y} \right) = 2A \cos \pi \cos k_{x_1} x$$

with $k_s = \sqrt{k_0^2 - (\pi/d_s)^2}$ and $k_0$ being the vacuum wave number. For electron guns, a symmetric accelerating field over the bunch dimensions is usually favored, since it enables bunches with symmetric properties. As will be seen later, the considered slot for the photoinjector laser and the injection of bunches with symmetric properties should coincide with the center of the transition region and in turn weaken the accelerating field. As a rule of thumb, setting $g \approx \lambda_e/10$, with $\lambda_e = 2\pi/k_e$, provides a proper compromise between the aforementioned effects. This leads to $g = 0.12$ mm for the example considered.

To design the layer thicknesses, we initially consider an ideal scenario, in which the effect of fringing fields, transverse fields, inhomogeneous fields among different layers, and the broad frequency spectrum of the excitation are neglected. In this case, an electron synchronized with the incoming pulse, will be affected by the following field:

$$E_z = -A \eta_i |\sin \omega t| = -E_{\text{max}} \eta_i |\sin \omega t|,$$

where $\omega$ is the center frequency of the pulse, and $\eta_i$ is a field scaling factor defined for each layer. Note that the accelerating field profile in the ultrafast gun is fundamentally different from the conventional cascaded cavity gun technology, where fields are also position dependent. The different field profiles lead to various advantages and shortcomings compared to conventional technologies, which will be the subject of future investigations. Due to Fresnel reflection at the two boundaries of the quartz ($n = 2.1$) wafers in the layers above the first one, and additional fringing field effects from adjacent layers, the maximum acceleration gradient is smaller than $E_{\text{max}}$ considered for the first layer. The former effect reduces the field in the interaction section to 0.87$E_{\text{max}}$. If we consider 10% degradation for the later effect, the following equation for $\eta_i$ leads to a reasonable estimate for the acceleration gradient in different layers:

$$\eta_i = \begin{cases} 
1 & i = 1 \\
0.8 & i > 1 
\end{cases}.$$  

The energy of an electron in terms of distance during the first five half-cycles for the considered example is shown in figure 4. The temporal energy change indicates that five layers are required to obtain 400 keV electron beam. Moreover, the highlighted points A–E represent the transition positions from one cycle to the next one. Therefore, the corresponding $z$ coordinates should coincide with the center of the transition region between each layer. The positions of points A–E in figure 4 are obtained as

$$\{ z_A, z_B, z_C, z_D, z_E \} = \{ 100, 320, 650, 1020, 1420 \} \mu \text{m}. $$

![Figure 3](image-url)  
(a) Interaction region, (b) focuser section (top-view), and (c) coupler section (side-view) and the incoming Gaussian beam with critical dimensions.
Figure 4. Energy of an electron versus traveled distance accelerated by the field evaluated from (3). Points A–E are highlighted as transition points between consecutive cycles.

Table 1. The design parameters for the 400 keV gun and the optimized ones after fine tuning.

| Parameter | Designed value | Fine-tuned value |
|-----------|----------------|-----------------|
| \((d_1, d_2)\) | (0.71, 0.71) mm | (0.71, 0.71) mm |
| \((d_1, d_2, d_3, d_4)\) | (80, 180, 290, 330, 360) \(\mu\)m | (80, 180, 290, 330, 360) \(\mu\)m |
| \(t\) | 40 \(\mu\)m | 40 \(\mu\)m |
| \(g\) | 120 \(\mu\)m | 120 \(\mu\)m |
| \((L_1, L_2, L_3, L_4)\) | (0, 450, 900, 1350, 1800) \(\mu\)m | (0, 400, 800, 1300, 1800) \(\mu\)m |
| \((\theta, \alpha)\) | (18.0, 18.0) deg | (18.0, 14.0) deg |
| \((\tau, w_{0y}, w_{0z})\) | (3.33 ps, 1 mm, 1 mm) | (3.33 ps, 1 mm, 1 mm) |
| \(f\) | 300 GHz | 300 GHz |
| \(\varepsilon_i\) | 200 \(\mu\)J | 200 \(\mu\)J |
| \((x_p, y_p, z_p)\) | (±2.4, 0, 0.7) mm | (±2.7, 0, 0.64) mm |

If we assume \(t = 40 \mu\)m thick separators, the corresponding thickness of each layer reads as \(\{d_1, d_2, d_3, d_4\} = \{80, 180, 290, 330, 360\} \mu\)m. (5)

Now that the interaction section is designed, it is straightforward to estimate the required amount of energy for the presumed acceleration. The power propagating in a TE01 mode of a rectangular waveguide is obtained from:

\[
P = \frac{E_0^2}{2\eta_0} \frac{d_1 d_2}{2} \sqrt{1 - \left(\frac{\lambda}{2d_1}\right)^2},
\]

where \(\eta_0\) is the intrinsic impedance of free space, \(\lambda\) is the operation wavelength, and \(E_0\) stands for the maximum electric field in the waveguide. For the designed dimensions, i.e. \(d_i = \lambda/\sqrt{2}\) and \(E_0 = E_{\text{max}}/2\), the power flow of each mode can be obtained from \(P = E_{\text{max}}^2 \lambda d_i/32\eta_0\). If we neglect the dispersion in coupler and focuser and the resultant broadened pulse, the total energy due to each beam reaching the interaction region can be estimated as

\[
E = P\tau \sqrt{\frac{\pi}{4 \ln 2}} = \frac{E_{\text{max}}^2 \lambda d_i}{32\eta_0} \sqrt{\frac{\pi}{4 \ln 2}},
\]

with \(\tau = 1/f\) being the pulse duration of the single-cycle pulse. For the considered example in this section, the energy due to each beam in each layer is evaluated as

\[
(E_1, E_2, E_3, E_4) = (9, 19, 31, 35, 38) \mu\text{J}.
\]

Therefore, total energy of \(E_i = 132 \mu\text{J}\) should be coupled into the interaction region from each side to realize the desired acceleration.

The obtained value for \(E_i\) represents an estimate for the total amount of energy interacting with electrons. Several effects in the coupling and focusing process contribute to the energy loss before reaching the interaction region. The most dominant ones are reflection from thick separators in the coupler and intense pulse broadening due to dispersion in the focuser and coupler. Note that in the above calculation the Fresnel losses are taken into account, where \(E_0 = E_{\text{max}}/2\) is considered in all layers. According to our experience, 50% more energy is usually needed to realize the acceleration gradients assumed in each layer. In other words, two 200 \(\mu\)J energy beams should excite the ultrafast electron gun to realize 400 keV energy gain. This dramatic loss in energy motivates utilization of advanced coupling and focusing techniques instead of the simple horn couplers considered in this study.

Designing the focusing section revolves around determination of the length of dielectric inclusions and the horn angle, \(\theta\), in figure 3(b). The length of dielectrics are obtained from the difference in arrival time between two neighboring layers, which should be equal to \(\tau/2\). If we again neglect the dispersion effects of the waveguide, the values of \(L_i\) can be recursively obtained from the following equation:

\[
L_i = L_{i-1} + \frac{ct}{2(n - 1)},
\]

with \(n = 2.1\) being the quartz refractive index. As observed in figure 3(b), the quartz inclusions are assumed to be curved on one side. This curvature assists in better coupling of the input energy, since the beam portions close to the walls need to travel a longer path to reach the end of the focuser. Obtaining the best radius of curvature is an optimization problem and according to our experience, a curved surface which is perpendicular to the side walls at both ends is close to optimum.

An optimum value for \(\theta\) strongly depends on the spatial profile, i.e. the beam size, of the incoming Gaussian beam. More accurately, this angle should match with the divergence angle of the beam. Generally, beam confinement in vacuum using optical elements introduces considerably smaller dispersion to the pulse format compared with waveguides. This effect becomes even more important when propagation of a single-cycle pulse is involved. Therefore, it is always advantageous to focus the single-cycle beam close to its diffraction limit, namely \(w_0 = \lambda\), before entering the coupler. In
this case, the divergence angle of the Gaussian beam and consequently the horn angle $\theta$ is equal to $18^\circ$. Eventually, based on the same hypothesis the coupler angle $\alpha$ in figure 3(c) is similarly set to $18^\circ$. As will be seen in section 5, there exist cases where the length of the interaction region is larger than one wavelength. In such cases, the incoming Gaussian beams are focused to $w_0 > \lambda$ beam sizes for optimum coupling to the interaction region. The total length of the coupler ($L_c$) and focuser ($L_f$) does not play a significant role in the device operation. It is merely important to keep both lengths as small as possible in order to minimize the pulse broadening effect. However, both dimensions should be long enough to provide large enough aperture for capturing the total power of the Gaussian beam.

The explained profile matching condition additionally suggests the optimum position for the beam focus. The transverse dimension of the coupler should match with the beam size at the focus point. Since a much stronger focusing is desired in $xy$ plane, we consider the beam size as well as the structure dimensions along $y$ axis to determine the focal point of the excitations. This assumption yields $x_f = \pm 2.4$ mm for the optimum focal point in the 400 keV gun. In addition, $y_f = 0$ and $z_f = 0.7$ mm maintains a symmetric excitation along $y$ axis and distributes energy uniformly among different layers.

When all device and excitation parameters are determined, we can simulate the described device and assess the design obtained through the initial optimization process. All the dimensions of the electron gun as well as the excitation beam are tabulated in table 1. The fields are evaluated using an in-house developed time domain Maxwell solver based on the discontinuous Galerkin time domain technique [41]. Next,

Figure 5. Simulation results of the initial design for the 400 keV electron gun: (a) accelerating field in the middle of each layer versus time, and (b) energy of an electron injected at the 33.6 ps time instant versus traveled distance.

Figure 6. Simulation results of the optimized design for 400 keV electron gun: (a) accelerating field in the middle of each layer versus time, and (b) energy of an electron injected at instant with 80 MV m$^{-1}$ accelerating field.
the proper injection time of one electron is extracted from the field temporal variations in the first layer. The electron energy gain and trajectory within the simulated fields are then computed using a particle-in-cell algorithm [41]. In figure 5, the temporal signatures of the accelerating field at the center of each layer and the electron energy versus time are depicted as outcomes of the simulation. It is seen that the design process in spite of neglecting many influential effects results in a function close to the target operation. The sensitivity analysis presented in [36] demonstrates operational stability even after 10% changes in the parameter values, which is a result of the single-cycle, i.e. broadband operation of the device. As a consequence, finding the values for an operating electron gun is a straightforward task. However, the required transient simulations introduce serious challenges during device optimization.

| Parameter | Ultimate value |
|-----------|----------------|
| $(d_1, d_2)$ | (0.71, 0.71) mm |
| $(d_3, d_4, d_5, d_6, d_7, d_8)$ | (80, 180, 280, 320, 360, 390, 420, 450) μm |
| $t$ | 40 μm |
| $g$ | 120 μm |
| $(L_1, L_2, L_3, L_4, L_5, L_6, L_7, L_8)$ | (0, 400, 850, 1300, 1800, 2250, 2700, 3150) μm |
| $(L_p, L_c)$ | (3.5, 2.5) mm |
| $(\theta, \alpha)$ | (20.0, 14.0) deg |
| $(\tau, w_{10z}, w_{10y})$ | 2.1 (quartz) |
| $(f, w_0, w_0, f)$ | (3.33 ps, 1 mm, 2 mm) |
| $\varepsilon_r$ | 300 GHz |
| $\varepsilon_{\gamma}$ | 400 μJ |
| $(x_0, y_0, z_0)$ | (±2.4, 0.0, 1.34) mm |

Figure 7. Acceleration of 1 pC photoemitted bunch in the fine-tuned 400 keV THz gun: (a) mean energy and energy spread of the bunch, (b) bunch charge, (c) bunch length and (d) bunch size at the gun exit are depicted in terms of the traversed distance.
4. Fine tuning

As previously emphasized, the described process for the initial design is neglecting several effects. To acquire an optimum operation, fine tuning of the dimensions is an indispensable task. Owing to the computationally demanding full-vector simulations needed to verify each set of parameters, this effort is very time consuming. However, scrutiny of the field and electron energy variations considerably reduces the expense for fine tuning and optimizing the gun performance.

For example, it is observed that the time delay between the accelerating cycles in the first and second layers are longer than expected (figure 5(a)). Therefore, to correct this time delay the length of the dielectric inclusion in the second subwaveguide, i.e. \( L_2 \), should be reduced. Once this time delay is corrected, the lengths \( L_1 \) in sub-waveguides of the upper layers should be similarly reduced to maintain the synchronization of electrons with the pulse front. In addition, care must be exercised when injecting one single electron and optimizing the acceleration scheme. In practice, a bunch over an extended time will be injected into the device. Hence, injecting electrons at the zero-crossing, as done in figure 4, incurs losing almost half of the photoemitted electrons. To avoid this effect, the center of the bunch must experience the field with a phase larger than zero. This results in losing a fraction of the input beam and smaller optimum thickness of the gun layers.

Continuous acceleration between the layers may initially be envisaged and favored to maximize the energy transfer from the THz beam to the electrons. However, this leads to a concomitant increase in energy spread of the output bunch. To reduce the energy spread, it is advantageous to impose time delays between layers which are slightly larger than a half cycle. This assumption causes higher energy electrons in front of the bunch gain less energy than the ones in the back, which in turn reduces the ultimate energy spread. For this purpose, thick separators between acceleration layer enable more efficient velocity bunching compared with thinner ones. Similar subtleties exist in the coupling mechanism of the Gaussian beam. The presented qualitative measures for setting the angle of horn couplers and focus position of the beam are based on the beam waist \( (w_0) \), which encompasses around 86% of the total incident power. More efficient coupling is obtained by accounting for a larger effective spot size, while determining the values of \( \alpha, \theta, \) and \( (x_f, y_f, z_f) \).

After improving the design based on the above considerations and performing a series of iterative optimization on the various involved parameters, the values tabulated in table 1 in conjunction with the updated field signature and electron energy gain depicted in figure 6 are obtained. The new results evidence a pronounced enhancement in the device operation through the fine tuning procedure. We comment that the energy gain in figure 6 is obtained for one electron injected at the time when the accelerating field is 80 MV m\(^{-1}\), which demonstrates acceleration up to 400 keV electron energy.

It is often helpful for the design process to define a figure of merit for the performance. A suitable measure is the ratio of energy gain for one electron to the total input energy. For instance, the fine-tuned device results in the ratio \( 1.0 \text{ keV } \mu J^{-1} = 1.59 \times 10^{-10} \), while the initial design leads to the ratio \( 0.92 \text{ keV } \mu J^{-1} = 1.48 \times 10^{-10} \). Note that this measure verifies the overall coupling, focusing and acceleration schemes with the exclusion of bunch evolution. Another measure to separately assess the coupling and focusing sections can be defined as the ratio between the energy of one cycle with maximum field in the interaction region to the total input energy. The nominator is obtained in a similar fashion as (7), but with the ultimate maximum

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**Figure 8.** Simulation results of the optimized design for 800 keV electron gun: (a) accelerating field in the middle of each layer versus time, and (b) energy of an electron injected at the instant with 200 MV m\(^{-1}\) accelerating field.
acceleration gradients ($E_i$), and the denominator is simply the input energy of the Gaussian beam ($\varepsilon_i$). Therefore, this ratio can be written as

$$\mathcal{R} = \sum_i \frac{E_i^2 \lambda d_i}{32 n_0 \varepsilon_i} \sqrt{\frac{\pi}{4 \ln 2}}.$$  \hspace{1cm} (10)

This ratio for the fine-tuned device and the initial design are obtained as 0.47 and 0.46. In other words, although the fine tuning enhanced the total acceleration scenario, it only slightly varied the coupling of the THz beam. This has occurred because of the strong interdependence between all the involved parameters in the overall performance. Examining the above introduced parameters for each design properly guides the fine tuning process of the electron gun dimensions.

After optimization and finalizing the design for acceleration of a single particle, a more accurate assessment of the structure is achieved through investigation of the full bunch acceleration scenario. For this purpose, we assume a copper cathode excited by a UV laser pulse at 250 nm wavelength with full-width half-maximum (FWHM) pulse duration equal to 47 fs and FWHM spot size diameter 47 $\mu$m. The UV laser energy is supposed to be large enough such that 1 pC of charge is released, which is modeled by 20,000 macro-particles. The 6D phase-space distribution of such a photocathode is obtained using the ASTRA bunch generator module. In addition, we use a point-to-point algorithm to account for Coulomb repulsion between electrons, i.e. space-charge (SC) effects.

Figure 7 shows the evolution of the bunch properties throughout the acceleration process. The bunch parameters are depicted for the two cases with and without consideration of SC effects. The bunch parameters obtained without SC are valid in the low-charge regime ($<100$ fC), whereas acceleration
of 1 pC injected charge suffers from strong SC forces that increase position and energy spread. It is observed that the final mean energy of the bunch is about 390 keV with an energy spread of about 1.5%, which happens due to the large spot size of the injected bunch compared to the THz wavelength (1 mm) and SC forces. The compensation of energy spread when the bunch traverses the separators can be seen in figure 7(a). This effect is the main advantage of thick separators enabling velocity bunching in this region. Due to the collisions of the electrons with the metallic boundaries emanating from the transverse momentum of electrons, 73% of the photoemitted electrons are extracted from the gun. This effect shows the limitation on bunch size and correspondingly the amount of charge which can be accelerated with a desirable quality using the proposed THz gun.

The normalized emittances of the beam at the output with and without SC are evaluated as \( \epsilon_{x, y, z} \) = (0.20, 0.25, 0.21) mm mrad and (0.17, 0.13, 0.11) mm mrad, respectively.

5. 800 keV gun

The described design procedure, as used for designing an exemplary 400 keV gun, can be generally followed to design any type of gun excited with short pulses in THz and microwave regimes. An electron gun with 400 keV output energy may be a suitable option for applications like electron diffractive imaging. However, for injecting to a linear accelerator, where velocity matching with the phase of the accelerating field is essential, electron guns with higher output energies are required. In what follows, the design for an optimum 800 keV electron injector is given following the same design procedure. The 800 keV gun consists of eight layers in the interaction section with design parameters tabulated in table 2.

The results of the single particle acceleration simulation are depicted in figure 8. As demonstrated by the simulations, by just adding three layers and doubling the beam input energy, the energy gain of the particles is doubled to 820 keV. We comment that in this example the incident Gaussian beam is considered to be elliptical to better match with the acceleration length, which is relatively long in comparison with the transverse size of the interaction section. In practice, such an elliptical Gaussian beam is realized using standard optical elements. Otherwise, the coupler parameters need to be adjusted based on the input Gaussian beam dimensions. According to these results, the ratio between energy gain for one electron and the total input energy is equal to 1.03 keV \( \mu \text{J}^{-1} = 1.65 \times 10^{-10} \), which is slightly better than for the 400 keV gun and additionally the \( R \) parameter defined in (10) is calculated as 0.52. Eventually, the bunch acceleration is inspected by injecting the same photoemission electron bunch as in the 400 keV gun study. The results of this analysis are illustrated in figure 9, which demonstrates realization of a 520 fC electron beam with 811 keV mean energy, 1.2% energy spread, and bunch dimensions of about (25 \( \mu \text{m} \times 58 \mu \text{m} \times 16 \mu \text{m} \)). The output normalized emittances are evaluated as \( \epsilon_{x, y, z} \) = (0.13, 0.69, 0.43) mm mrad for the SC included simulation and \( \epsilon_{x, y, z} \) = (0.09, 0.29, 0.15) mm mrad without accounting for SC effects. In addition, the transverse beam profile and longitudinal phase-space of the electron bunch at the output of the gun including SC effects are illustrated in figure 10.

6. Conclusion

We have presented a systematic procedure to design and optimize an ultrafast electron gun driven by single-cycle THz pulses. Based on the described process, a 400 keV five layer
THz gun is designed which utilizes two 200 μJ single-cycle pulses at 300 GHz to realize a maximum acceleration gradient of about 650 MV m⁻¹ at the cathode surface. The output of the gun is a 0.75 pC electron bunch with 50 fs pulse duration and emittances in the range of 0.1 mm mrad. Such a design demonstrates that single-cycle ultrafast electron guns can generate the required electron beams for electron diffractive imaging using the currently available THz sources. Subsequently, an upgraded THz gun with three more layers is presented, which is fed by two 400 μJ pulses and which boosts the energy gain to 810 keV. The SC effect is the dominant factor causing particle loss, when pC-level bunches are injected into the gun. Due to this effect, the charge yield of the 800 keV electron gun is about only 50% or only 0.52 pC bunches are generated from the gun. The energy of the electrons produced by this gun is sufficiently high to be injected into electron linacs.

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