Multiobjective optimization design of an rf gun based electron diffraction beam line

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Multiobjective genetic algorithm optimizations of a single-shot ultrafast electron diffraction beam line comprised of a 100 MV/m 1.6-cell normal conducting rf (NCRF) gun, as well as a nine-cell $2\pi/3$ bunching cavity placed between two solenoids, have been performed. These include optimization of the normalized transverse emittance as a function of bunch charge, as well as optimization of the transverse coherence length as a function of the rms bunch length of the beam at the sample location for a fixed charge of 10^6 electrons. Analysis of the resulting solutions is discussed in terms of the relevant scaling laws, and a detailed description of one of the resulting solutions from the coherence length optimizations is given. For a charge of 10^6 electrons and final beam sizes of $\sigma_x \geq 25 \mu\text{m}$ and $\sigma_t \approx 5 \text{ fs}$, we found a relative coherence length of $L_{c,x}/\sigma_x \approx 0.07$ using direct optimization of the coherence length. Additionally, based on optimizations of the emittance as a function of final bunch length, we estimate the relative coherence length for bunch lengths of 30 and 100 fs to be roughly 0.1 and 0.2 nm/ μm , respectively. Finally, using the scaling of the optimal emittance with bunch charge, for a charge of 10^5 electrons, we estimate relative coherence lengths of 0.3, 0.5, and 0.92 nm/ μm for final bunch lengths of 5, 30 and 100 fs, respectively.

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I. INTRODUCTION

The desire for single-shot ultrafast electron diffraction (UED) beam lines with sufficient resolution ($\sigma_t \lesssim 30 \text{ fs}$, $q \sim 10^6$ electrons) for use with biological samples, such as proteins, continues to push the development of both photocathode and cold atom electron sources [1–17]. For photoemission UED sources such as DC and normal conducting rf guns (NCRF) [18], the charge and beam sizes at the cathode require optimal emittance preservation of a space charge dominated beam. Building on the successful application of multiobjective genetic algorithm (MOGA) optimized simulations of space charge dominated beams used in the design and operation of the Cornell photoinjector [19–21], as well as the optimization of a cryocooled DC gun UED setup [22], we apply the same techniques to a 100 MV/m 1.6-cell NCRF gun followed by a nine-cell, $2\pi/3$ buncher cavity. We use a mean transverse energy (MTE) of 35 meV for the simulated photoelectrons, a value considered achievable through the use of multialkali photocathodes operated near threshold [23].

The NCRF gun based UED setup in this work consists of a 1.6-cell 2.856 GHz NCRF gun followed by a buncher cavity placed between two solenoid magnets [24–26]. For all simulations, the maximum allowable peak cathode field is set to 100 MV/m and the cathode MTE is fixed to 35 meV for all simulations. For the buncher model, we used the dimensions of the first cell in the SLAC linac [27] (see Table I) repeated a total of 9 times, to make a nine-cell $2\pi/3$ traveling wave buncher cavity. The field maps were generated in Poisson SUPERFISH [28].

To model solenoids similar to those in [24,25] we use an analytic form for the on-axis solenoid field from a sheet of current with radius R and length L ,

$$B_z(z) = B_0 \left(\frac{\Delta z_+}{\sqrt{\Delta z_+^2 + R^2}} - \frac{\Delta z_-}{\sqrt{\Delta z_-^2 + R^2}} \right), \quad (1)$$

where $\Delta z_{\pm} = z \pm L/2$ and fit this model to solenoid field map data [22]. The fields used in space charge simulations are computed from the third order off-axis expansion of Eq. (1). Figure 1 shows the on axis field data for the beamline setup.

II. RESULTS

For this work, we make use of the same MOGA software used in previous work [19,20,22] in combination with the 3D space charge code general particle tracer (GPT). In each

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TABLE I. Buncher cavity design parameters.

Parameter	Value
Period d	3.5 cm
Cell diameter $2b$	8.34 cm
Disk hole diameter $2a$	2.62 cm
Disk thickness t	0.58 cm
Disk edge radius ρ	0.31 cm

optimization, the optimizer was allowed to vary the laser rms sizes, beam line element parameters and positions, as well as arbitrarily shape both the transverse and longitudinal laser distributions, based on the same methods described in [22,29]. The set of beam line parameters varied are shown in Table II. In all optimizations the population size was set to 50. The number of generations run for each optimization ranged between several hundred to a several thousand, depending on whether the optimization was starting from noise or being seeded from a previous solution. Progression of the front was monitored every 10 to 20 generations after an initial 200. When no discernible improvement of the front was found, the optimization was stopped.

A. Optimal emittance

Fundamentally, for a given bunch charge, the coherence length at the sample is limited by the cathode emittance produced in the charge saturation limit, as well as the ability to preserve this emittance while transporting and focusing the beam down to the required beam sizes at the sample [22]. For a given charge q extracted in the charge saturation limit for an accelerating field E_0 , the limiting emittance scales as

$$\epsilon_{n,x,i} \propto \sqrt{\frac{\text{MTE}}{m_e c^2}} \begin{cases} \left(\frac{q}{\epsilon_0 E_0}\right)^{1/2}, & A \gg 1 \text{ ("pancake")} \\ \frac{1}{E_0} \left(\frac{q}{\sigma_{t,i}}\right)^{2/3}, & A \leq 1 \text{ ("cigar")}. \end{cases} \quad (2)$$

TABLE II. Beam line simulation parameters.

Parameter	Range
Laser size $\sigma_{t,i}$	[0, 20] ps
Laser size $\sigma_{x,i}$	[0, 1] mm
Cathode MTE	35 meV
Peak gun field	100 MV/m
Gun phase	[0, 360] deg
Solenoid radius/length	2.53/9.54 cm
Solenoid peak field(s)	[0, 1.0] T
Solenoid 1 position	[0.25, 5.25] m
Peak buncher power	[0, 25] MW
Buncher phase	[0, 360] deg
Buncher position	[0.4, 10.4] m
Solenoid 2 position	[0.55, 15.55] m
Sample position	[0.55, 20.55] m

(a) Example of the on-axis accelerating (blue) and solenoid field profiles (green).

FIG. 1. Field description for the 1.6-cell gun and solenoid (a), as well as the buncher (b).

In this expression $\sigma_{t,i}$ is the rms laser pulse length, and $A = \sigma_{x,i} / \left(\frac{eE_0}{m_e c^2}\right) (c\sigma_{t,i})^2$ is the initial beam aspect ratio. Note the limit $A \ll 1$ describes the short initial bunch regime.

To verify the validity of Eq. (2), we performed an initial round of emittance optimizations for a “long” final beam $\sigma_t \leq 500$ fs (the bunch length is also minimized later), while constraining the transverse spot size: $\sigma_x \leq 25 \mu\text{m}$, and simultaneously maximizing the bunch charge. In these optimizations, we require that no particles are lost in beam transport. Figure 2 shows the emittance performance. The figure also shows the results of fitting the emittance data with both charge scaling laws found in Eq. (2) for beams extracted in the charge saturation limit, and suggests that the emittance at the sample scales as $q^{2/3}$. Noting that the optimizer chose an initial laser pulse length of roughly 2.4 ps for the charges shown, and computing the initial beam aspect ratio for all points on the front leads to an

FIG. 2. Optimal emittance as a function of bunch charge at the sample for a final beam size of $\sigma_x \leq 25 \mu\text{m}$, $\sigma_t \leq 500$ fs.

FIG. 3. The optimal emittances as a function of bunch length for a final beam size of $\sigma_x \leq 25 \mu\text{m}$ (blue) and $\sigma_x \leq 100 \mu\text{m}$ (red), respectively.

aspect ratio range of roughly 0.006 to 0.1, verifying the fitted scaling law.

With these results, we fixed the charge to 10^6 electrons and reoptimized, this time minimizing the emittance as a function of bunch length. Figure 3 shows the results for two final beam spot sizes at the sample: $\sigma_x \leq 25$ and $100 \mu\text{m}$ and demonstrates that the emittance scales weakly with spot size for final beam sizes of $\sigma_x \geq 25 \mu\text{m}$. Additionally, the data shows the emittance scales weakly with the final bunch length down to roughly $\sigma_t \sim 100$ fs. For shorter bunch lengths the emittance suffers, though we note the existence of feasible solutions with small emittances $\epsilon_{n,x} \lesssim 5$ nm for bunch lengths as short as $\sigma_t \sim 5$ fs. Note, for this plot and all similar ones, we fit a rational polynomial to the Pareto front in order to better guide the eye and to aid estimating and interpolating between points on the front. The dashed black line in this plot indicates where the optimizer selected initial rms laser sizes corresponding to an initial beam aspect ratio of $A \approx 0.5$. Beams to the right of this line are considered to be created in the

FIG. 4. Optimal coherence length as a function of bunch length at the sample for a final beam spot size of $\sigma_x \leq 25 \mu\text{m}$.

TABLE III. Average optimized beam line element positions.

Element	Position
Solenoid 1	0.25 m
Buncher cavity	0.48 m
Solenoid 2	1.07 m
Sample pinhole	2.63 m

long pulse regime. It is instructive to also estimate the disordered induced heating (DIH) of the beam for this data. To do so we assume a uniform beam with equivalent rms sizes. From this, the volume of the beam after being emitted from the cathode follows:

$$V = \pi R^2 L \approx \pi (2\sigma_x)^2 \cdot \frac{1}{2} \frac{eE_0}{m} (\sqrt{12}\sigma_t)^2 \approx \frac{24\pi E_0}{mc^2 [\text{eV}]} \sigma_x^2 (c\sigma_t)^2. \quad (3)$$

From this we estimate the effect of DIH using the formula given by Maxson: $\Delta kT [\text{eV}] = 1.04 \times 10^{-9} (n_0 [\text{m}^{-3}])^{1/3}$ [30], where n_0 is the electron number density. For the shortest final bunch lengths, the DIH estimate is roughly 150 meV. Since this heating occurs near the cathode, this would correspond to roughly a factor of $\sqrt{150/35} \approx 2$ increase in the emittance, and would subsequently reduce the coherence length by a factor of 2. It is important to note that this estimate may indicate that DIH will be important, however, the true estimate of the effect depends on the detailed dynamics of the initial expansion of the beam, and lies beyond the scope of this work.

B. Optimal coherence length

Using the emittance vs bunch length solutions for a final spot size of $25 \mu\text{m}$ in Fig. 3 as a seed, optimizations for the maximum transverse coherence length were performed.

FIG. 5. Optimal beam line element positions for a final beam spot size of $\sigma_x \leq 25 \mu\text{m}$.

FIG. 6. Transverse (a) and longitudinal (b) rms beam size along the beam line, as well as the transverse emittance (c). Insets show the transverse (a) and longitudinal (b) beam distributions and (c) transverse phase spaces at the cathode and sample locations.

Figure 4 shows the optimal coherence length as a function of the final bunch length σ_t , constrained so that $\sigma_x \leq 25 \mu\text{m}$. In particular, the data shows a relative coherence length of $L_{c,x}/\sigma_x \approx 0.07 \text{ nm}/\mu\text{m}$ for a final bunch length of $\sigma_t \approx 5 \text{ fs}$. While the optimizer did not choose solutions at longer bunch lengths in this optimization, using the emittance data in Fig. 3 and the expression for the coherence length at beam waist, $L_{c,x} = \lambda\sigma_x/\epsilon_{n,x}$, we

estimate the relative coherence length at 30, 100, and 500 fs to be 0.1, 0.2, and 0.3 $\text{nm}/\mu\text{m}$, respectively. This implies $L_{c,x}(\sigma_t \rightarrow 500 \text{ fs}) \rightarrow 8 \text{ nm}$, as displayed in the figure. It is instructive to compare these results to those found in [26]. At roughly the same bunch length (5 fs), the relative coherence from Han is about 0.014 $\text{nm}/\mu\text{m}$, implying a factor of 5 improvement in our results. We note, however, that an MTE of 600 meV and a max

accelerating field of 80 MV/m were used in [26]. Accounting for these differences would bring the relative coherence length in [26] up to 0.07, in agreement with this work. Thus, we point out the majority of the improvement comes from using a better cathode MTE.

In addition to determining the optimal coherence length, the optimizations producing the data in Fig. 4 also provide information about the optimal positioning of the beam line elements in each setup. Table III displays the element positions averaged over the optimization data shown in Fig. 5.

C. Example solution

In order to get a better feel of the beam dynamics determined by the coherence length optimizations, we ran a single example solution from the coherence vs final bunch length fronts shown in Fig. 4. This solution has a kinetic energy of 4.5 MeV, typical of all of the simulations presented in this work. Table IV displays the resulting relevant beam parameters. Of note are the initial laser sizes of $\sigma_{x,i} \approx 5 \mu\text{m}$ and $\sigma_{t,i} \approx 32 \text{ fs}$. These correspond to an initial beam aspect ratio of roughly 4×10^4 . We note that though the optimizer did not generate solutions here at longer bunch lengths, the optimal emittance results suggest viable solutions for longer bunches do exist. Figure 6(a) shows the transverse rms beam size along the beam line, as well as the initial transverse laser profile and the final electron transverse distribution at the sample. The optimizer chose a roughly flat-top transverse laser profile with $\sigma_x \approx 5 \mu\text{m}$. Figure 6(b) shows the rms bunch length, and the initial temporal current profile produced by the laser, and the electron beam current profile at the sample. The use of the buncher cavity allows for a fairly constant bunch length along the beam line up to the cavity, where the buncher applies an energy chirp which results in the bunch being compressed by the time it reaches the screen. The relevant emittance data along the beam line is shown in Fig. 6(c). Shown in solid blue is the transverse emittance with the angular velocity due to the solenoid removed.

TABLE IV. Example parameters and results.

Parameter	Simulated value
q	10^6 electrons
Gun phase (from peak field)	-47 deg
Buncher phase (from on-crest)	-90
Buncher peak power	22.5 MW
Laser $\sigma_{x,i}$	$4.68 \mu\text{m}$
Laser $\sigma_{t,i}$	32 fs
Aspect ratio A	4×10^4
KE	4.5 MeV
σ_x	$\leq 25 \mu\text{m}$
σ_t	5 fs
$\epsilon_{n,x}$	5.2 nm
$L_{c,x}$	1.85 nm

Shown in green is the slice emittance, computed by averaging over the (30) individual slices. As anticipated, the individual slice phase spaces are nearly aligned at the sample.

III. CONCLUSION

In this work, we have presented a multi-MeV NCRF gun based single-shot UED layout determined by MOGA optimization of space charge simulations. For a long final bunch of 500 fs or less, the emittance for this setup scales as $q^{2/3}$, in agreement with the predictions for a long initial beam aspect ratio [24,25]. Emittances as low as 2–5 nm were found for final bunch lengths ranging from roughly 500 fs down to 5 fs for a bunch charge of 10^6 electrons. In addition to computing the optimal emittances as a function of bunch length, optimizations of the coherence length as a function of the final bunch length produced coherence lengths suitable for single-shot UED experiments with a final electron beam spot size of $\sigma_x \geq 25$ and bunch charge of $q \leq 10^6$ electrons. In particular, direct optimization of the coherence length produced relative coherence lengths as low as 0.07 nm/ μm for a final bunch length of $\sigma_t \approx 5 \text{ fs}$. Estimating the relative coherence length using optimal emittance data for final bunch lengths of 30 and 100 fs yields relative coherence lengths of 0.1 and 0.2 nm/ μm , respectively. Based on the $q^{2/3}$ scaling demonstrated in the optimal emittance results, we estimate a factor of 4.6 improvement in the relative coherence numbers (0.3, 0.5, and 0.92 nm/ μm respectively) if the bunch charge was reduced to 10^5 electrons.

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