Improvement of 6D brightness by a 1.4-cell photocathode RF gun for MeV Ultrafast electron diffraction

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Abstract. Recent research indicates that ultrafast electron diffraction and microscopy (UED/M) have unprecedented potential in probing ultrafast dynamic processes, especially in organic and biological materials. However, reaching the required brightness while maintaining high spatiotemporal resolution requires new design of electron source. In order to produce ultrashort electron beam with extreme high brightness, a 1.4-cell RF gun is being developed to reach higher acceleration gradient near the photocathode and thus suppress the space charge effect in the low energy region. Simulation of the 1.4-cell RF photocathode gun shows considerable improvement in bunch length, emittance and energy spread, which all lead to better temporal and spatial resolution comparing to traditional 1.6-cell RF photocathode gun. The results demonstrate the feasibility of sub-ps temporal resolution with normalized emittance less than 0.1 πmm·mrad while maintaining 1 pC electron pulse.

1. Introduction

Over the past decade, ultrafast electron diffraction and microscopy (UED/M) based on laser-driven photocathode RF gun opens new possibilities to investigate nano-structure dynamics within sub-ps temporal resolution [1, 2]. Institutions around the world has shown successful observation of dynamic process of structures like single crystal [3], organic salt crystal [4], amyloid [5], etc. with temporal resolution ranging from ns to fs. Based on these current researches, we believe if we push the 6D brightness to a new level and thus achieve higher signal to noise ratio and spatiotemporal resolution, it will be possible to observe and record the ultrafast process of more complicated materials such as proteins, DNA molecules, or even living cells [6].

To improve the 6D brightness of electron beam, UCLA firstly proposed to use 1.4-cell RF gun, instead of more commonly used 1.6-cell RF gun, to increase the optimal injection phase and thus increase the extraction field near the cathode [7]. Here optimal injection phase refers to the phase upon which beam achieves maximum energy. In our case of 3 MeV beam, the extraction field for the 1.4-cell RF gun is about 4.5 times higher than the 1.6-cell one. There are two main reasons why we believe higher extraction field could increase the 6D brightness. Firstly, according to current research of photoemission model, the maximum transverse brightness that can be achieved by the photocathode directly affected by the extraction field. For the pancake regime beam we use in UED/M experiment, the maximum transverse brightness is proportional to extraction field as shown in equation (1) [8]

\[ B_{max} \propto \frac{E_{cathode}}{kT} \]  

(1)
where $E_{\text{cathode}}$ is the extraction field on the cathode. Secondly, high brightness beam inevitably suffers from the space charge effect which is proportional to $1/\beta^2 \gamma^3$ [9]. With higher extraction field, electrons emitted from photocathode accelerate to near-relativistic region faster hence suppress the space charge effect. For the pancake beam, the dilation and degradation caused by space charge effect are mainly in the longitudinal direction, thus the beam produced by 1.4-cell RF gun should have smaller longitudinal emittance.

In this paper, we report the design of new 1.4-cell RF photocathode gun with SUPERFISH simulation. The comparison between the new gun and a standard 1.6-cell gun performed by ASTRA [10] are reported. Advantages in both transverse and longitudinal emittance under high charge density are observed which lead to approximately 5 times higher 6D brightness. Finally, we present the beam dynamics simulated by ASTRA to show the preliminary performance in the 1.4-cell RF gun. The simulation results indicate an ultrashort-pulsed electron beam with 210 fs rms bunch length and 0.08 $\pi\text{mm} \cdot \text{mrad}$ normalized emittance at 1 pC can be generated with the 1.4-cell RF gun.

2. 1.4-cell RF gun design

2.1. RF design

The resonant modes of this 1.4-cell RF gun are calculated by SUPERFISH. Figure 1 shows the cavity profile and electric field distribution of $\pi$-mode along the axis.

![Figure 1. 1.4-cell cavity and field distribution.](image)

The 1.4-cell cavities were fabricated and brazed at High Energy Accelerator Research Organization (KEK). Cold test indicated good agreement with simulation.

2.2. Compensating Solenoid

To evaluate the quality of beam produced by the RF cavity, we need to consider the effect of compensating solenoid. Here we introduce the model we used for all the simulation involving compensating solenoid in this paper. Figure 2 shows the on-axis field distribution of this model. The center of this solenoid model is placed 0.2 m away from the cathode. The leaking magnetic flux at cathode is less than 10 gausses after scaling, which is acceptable for ASTRA simulation.

![Figure 2. Solenoid field distribution.](image)

To compare the beam dynamics in both the 1.4-cell and a 1.6-cell RF guns, we use this same solenoid model in the simulations as described in the next section.

3. 1.4-cell & 1.6-cell comparison

The main difference between the 1.4-cell and 1.6-cell RF guns (referred as 1.4-cell and 1.6-cell for short) is the optimal injection phase for laser. The target beam energy for our UED operation is about 3 MeV. To reach this target energy for both RF guns, the optimal injection phase are 65.2° with a peak
field of 76 MV/m for 1.4-cell and 13.7° with 64 MV/m for a standard 1.6-cell. Hence, the effective extraction fields on cathode for two RF guns are

\[
E_{1.4} = 76 \cdot \sin(65.2°) \approx 67.2 \text{ MV/m} \\
E_{1.6} = 64 \cdot \sin(13.7°) \approx 15.2 \text{ MV/m}
\]

As we can see, the extraction field in 1.4-cell is about 4.5 times higher than that in 1.6-cell. To understand the suppression of the space charge effect with the higher extraction field, we proposed to scan the bunch charge from 0.05 pC to 1 pC with constant beam size to compare beam quality at different levels of space charge effect.

The distributions of laser pulse are Gaussian in three directions with \( \sigma_x=70 \mu \text{m} \) and \( \sigma_t=50 \text{ fs} \). The maximum magnetic flux \( B_{\text{max}} \) of solenoid is scaled accordingly to obtain parallel beam after the RF gun. The beamline ends at \( z=0.8 \text{ m} \) (\( z=0 \) for cathode) where approximately is the position of specimen holder. Beam parameters are all compared at this position.

**Figure 3.** Transverse(left) and longitudinal(right) emittance by 1.4 and 1.6-cell RF guns at 70 \( \mu \text{m} \) and 50 fs.

Figure 3 gives the transverse emittance and the longitudinal emittance as functions of bunch charge. As we can see in this case, the 1.4-cell RF gun shows clear advantage in longitudinal emittance at bunch charge of >0.2 pC. Transverse emittance is more difficult to decipher but we can conclude that two kinds of cavities share comparable transverse emittance.

In addition, the longitudinal emittance of 1.4-cell grows much slower than 1.6-cell as charge increases. This could be an evidence for better space charge effect suppression. The beam we used for both RF guns is pancake-shaped, which means the dilation caused by space charge effect is mainly in the longitudinal direction. Therefore, with better space charge suppression, the longitudinal emittance in 1.4-cell grows slower and remains a relatively small value in spite of its slightly larger value in the low charge region.

In UED/M operation, large longitudinal emittance usually corresponds to large bunch length and energy spread, resulting in loss of temporal and spatial resolutions.

**Figure 4.** Bunch length (left) and energy spread (right) generated by 1.4 and 1.6-cell RF guns at 70 \( \mu \text{m} \) and 50 fs.

Figure 4 shows the bunch length and energy spread generated by the 1.4 and 1.6-cell RF gun. Note that bunch length of 1.4-cell grows slower as bunch charge increases, which suggests 1.4-cell only
shows significant advantage in temporal resolution under severe space charge effect. 1.4-cell also shows slight yet consistent advantage in energy spread, which we suspect could be the result of its near-crest injection phase and shorter cavity length.

Combining above results, we calculated the 6D brightness in both the 1.4 and 1.6-cell RF guns as shown in Fig. 5. To avoid confusion of different conventions, we simply define 6D brightness as

$$B_{6D} = \frac{Q}{\epsilon_x\text{, norm}\epsilon_y\text{, norm}\epsilon_z\text{, norm}}$$

Although results in figure 5 may not stand for universal condition, it suggests that 1.4-cell has advantage at the bunch charge of >0.4 pC. A higher 6D brightness can be obtained with the 1.4-cell RF gun.

4. Beam dynamics of 1.4-cell RF gun

4.1. UED requirement

In UED operation, various parameters affect spatiotemporal resolution. To perform UED experiment, the diffraction patterns must be sharp enough to distinguish from each other, which requires transverse emittance less than 0.1 πmm·mrad. Energy spread causes different diffraction angle which also blurs the diffraction pattern. The ideal relative energy spread is less than 0.1%. RMS bunch length directly affect the temporal resolution of UED. To obtain sub-ps temporal resolution for UED operation, the ideal bunch length is less than 100 fs.

However, the transverse emittance, energy spread, and bunch length are coupling, which means it is unlikely for them to be minimum at the same time. A trade-off must be decided according to particular application.

4.2. Simulation result

The variables we can adjust including RF field amplitude, injection phase, laser spot size, laser pulse length, beam charge and solenoid field, etc. To achieve high signal-to-noise ratio for complicate biological materials, we choose 1 pC bunch charge which is more than enough for UED operation. After some scanning and iteration, we choose the initial parameters shown in table 1.

| Table 1. Initial Parameters. | Description | Parameters |
|-----------------------------|-------------|------------|
| RMS laser spot size         | $\sigma_{xy} = 80\mu m$ |
| RMS bunch length            | $\sigma_z = 40\, fs$ |
| Electrical field amplitude  | $E_z = 74\, MV \, /\, m$ |
| Injection phase             | $\phi=65^\circ$ |
| Maximum solenoid field      | $B_{max} = 0.12\, ST$ |
According to ASTRA simulation as shown in Fig. 6, we obtain 3 MeV beam with relative energy spread of 0.23%. Transverse emittance at specimen is already less than 0.1 πmm·mrad without aperture. The bunch length at specimen correspond to about 210 fs. Combining with jitters of other systems, a sub-ps temporal resolution is possible.

The energy spread and bunch length are not ideal for UED experiment. One can increase laser spot size to trade transverse emittance for smaller bunch length and energy spread meanwhile use an aperture before specimen to lower transverse emittance below 0.1 πmm·mrad. This plan is also considered and bunch length around 100 fs and energy spread less than 0.1% are obtained despite the aperture eliminates more than a half of the bunch charge.

Note that we use Gaussian distribution for the initial transverse beam profile. While Gaussian distribution is commonly used for laser system, it is not the ideal transverse profile for best beam quality because of its non-linear space charge force. Further efforts on laser shaping can be made to achieve even better beam quality, for example, uniform ellipsoidal bunch [11].

5. Conclusions
In this paper we first show the design of 1.4-cell photocathode RF gun we are developing. Then we compare the ASTRA simulation of this 1.4-cell RF gun with a standard 1.6-cell one. Beam produced by 1.4-cell RF gun shows clear advantage in longitudinal emittance under severe space charge effect which corresponds to smaller bunch length and energy spread. All these characters indicate improvement of 6D brightness and spatiotemporal resolution of UED. In the end, we present the preliminary beam dynamics simulation before specimen. The results indicate feasibility of sub-ps UED experiment with 1 pC electron bunch.

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