

Simulation of electron bunch compression for a megaelectronvolt ultrafast electron diffraction facility at the National Centre for Nuclear Research in Poland

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We present simulations of the acceleration and compression of electron bunches for megaelectronvolt ultrafast electron diffraction (MeV-UED) experiments planned at the National Centre for Nuclear Research in Poland (NCBJ). This compact MeV-UED facility, currently under construction, will consist of an electron photoinjector, a superconducting accelerating HZDR/RI-type cryomodule housing two TESLA cavities, and experimental chambers. Simulations demonstrated the feasibility of producing short electron bunches with a duration of a few femtoseconds for electron beam energies ranging from 2 to 5 MeV.

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I. INTRODUCTION

An ultrafast electron diffraction facility operating in continuous-wave (cw) mode with a beam energy range of a few MeV (MeV-UED) has great potential for uncovering phenomena occurring on spatiotemporal atomic scales [1]. Molecular “movies” of chemical bond breaking and evolution have already been created using this technique and presented in 2020 [2] and 2021 [3]. MeV-UED has also been applied to understanding molecular properties of water [4,5] and elementary excitations [6]. Most existing experiments achieve a time resolution of tens of femtoseconds. However, many processes relevant to material properties occur on shorter timescales. Producing electron bunches shorter than 10 fs would enable MeV-UED to explore new research areas.

The time resolution of UED experiments depends primarily on two factors: the arrival time jitter and the electron pulse duration. The arrival time jitter is mainly caused by pulse-to-pulse energy fluctuations of electron bunches. Reducing arrival time jitter below 10 fs presents significant challenges, requiring achromatic magnet lattice optics and sophisticated synchronization systems between radiofrequency (rf) sources and lasers. Despite these challenges, there are initial results showing a reduction of the time jitter to below 8 fs rms [7]. The main component of the overall resolution reported in that publication was dominated by a pulse duration of 15 fs rms.

In this work, we focus on minimizing the electron pulse duration. Existing MeV-UED facilities generate and accelerate electron bunches using photoinjectors; however, future concepts are expected to incorporate additional rf cavities to further push the limits of temporal resolution in MeV-UED [8]. While the main emphasis of this study is on investigating the limits of bunch compression, we also briefly examine how the accelerator configuration optimized for maximum compression performs in terms of arrival time jitter.

The MeV-UED facility, which is part of the PolFEL project¹ at the National Centre for Nuclear Research (NCBJ), follows this new concept, consisting of two phases. Both phases will combine a photoinjector with an accelerating HZDR/RI-type cryomodule housing two superconducting TESLA cavities [9,10].

In the initial phase, a 1.6-cell photoinjector operating at 2.999 GHz, designed at Max IV in Lund, will be used. This design follows the concept of injectors operating at Max IV [11,12], which demonstrate peak electric fields (E_p) up to 90 MV/m. Two high-purity copper injectors will be constructed in-house at NCBJ, in collaboration with the Max IV team.

In the second phase, a 1.6-cell superconducting radio frequency (SRF) photoinjector operating at 1.3 GHz will replace the Max IV photoinjector. The SRF injector, combined with the SRF cryomodule, will enable cw operation mode of the MeV-UED facility at NCBJ. Two SRF photoinjector prototypes, developed over a decade at DESY, recently demonstrated the expected performance, using both

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¹The current PolFEL project, which is under construction following the recent funding cut, includes the UED line presented here and the THz line, which will be presented shortly.

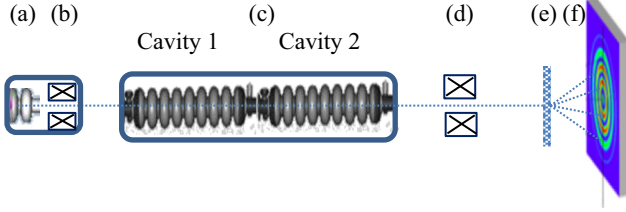


FIG. 1. Schematic layout of the MeV-UED beamline (not to scale), (a) electron source, (b),(d) solenoids, (c) accelerating cryomodule housing two cavities, (e) tested sample, and (f) detector.

superconducting niobium and normal-conducting copper cathodes [13,14]. Peak electric fields on both cathodes exceeded 56 MV/m at 2 K, significantly surpassing the 25 MV/m target for the NCBJ MeV-UED facility.

Figure 1 illustrates the beamline layout. Simulations confirm that this layout allows for generating very short electron bunches with durations of a few femtoseconds. The accelerating cryomodule provides additional flexibility to match beam properties to user requirements.

An electron bunch is generated and initially accelerated to an energy adjustable within the range of 2–4 MeV using one of the aforementioned photoinjectors.

The bunch then passes through the first solenoid before entering the superconducting accelerating cryomodule, where it is either accelerated or decelerated, depending on the beam energy required for the experiment. In this process, an energy chirp is obtained by appropriate rf phase adjustment. Afterward, the bunch passes through the second solenoid and drifts toward the sample, simultaneously undergoing ballistic compression. The second solenoid controls the beam's transverse size and convergence at the sample's location and the detector.

II. SIMULATIONS

We used the ASTRA package [15] to model the electron bunch generation, acceleration, shaping, and transport along the MeV-UED beamline. Owing to the cylindrical symmetry of the injectors, we employed two-dimensional modeling up to $z = 0.3$ m and three-dimensional modeling for $z > 0.3$ m, both using 10,000 macroparticles. The mirror charge was considered for $z \leq 0.3$ m, while the space charge was included for the entire trajectories in the simulation. Please note that only the x component of the beam emittance and the transverse beam size are displayed in the figures below for clarity, as the difference between the x - and y -components is negligible. The parameters and assumptions underlying the modeling are discussed below.

A. Photocathode and laser pulse parameters

Both types of photoinjectors will use metallic cathodes made of high residual resistance ratio copper or niobium.

TABLE I. Solenoids' parameters and positions.

Solenoid/injector	Length (m)	z_m (m)	$B_{\max}$ (T)
b/SRF	0.2	0.45	0.250
b/Max IV	0.24	0.32	0.092
d	0.44	10.52	0.170

The assumed quantum efficiency (QE) of the cathodes is 5×10^{-5} at 257 nm wavelength. This QE value is intentionally conservative and lower than the QEs demonstrated by the LCLS photoinjector at SLAC [16] and Tsinghua University in Beijing [17].

The output power of the purchased laser used to irradiate the cathodes is 2 W at 257 nm wavelength. For this study, we assumed a maximum bunch charge (q) of approximately 100 fC, which is delivered to the MeV-UED experiments.

The cw SRF injector will initially operate at 50 kHz repetition rate. To generate the 5 nA beam ($I_b = 100 \text{ fC} \times 50 \text{ kHz}$), a laser power of 0.48 mW will be required. The laser power will be significantly lower for the Max IV warm injector, operating in pulse mode at 100 Hz repetition rate. The repetition rate is currently limited by the existing laser system but could be further upgraded to reach the MHz range for the SRF injector.

The temporal profile of the laser pulse was assumed to be Gaussian, with a full width at half maximum (FWHM) duration of 250 fs ($\sigma_t = 106$ fs). The spatial transverse profiles of the laser pulse were also assumed to be Gaussian, with FWHM diameters of $\Phi = 10, 20, 25, 28, \text{ and } 50 \mu\text{m}$. The Gaussian shape was truncated in both time and space at $2\sigma_t$ and $2\sigma_x$, respectively.

B. Beam energy and solenoids

We studied two electron beam energies of 2 and 5 MeV at the sample. Nominal $B_{\max}$ of solenoids and distances, z_m , of their midplanes to the cathode are listed in Table I. Note that different versions of solenoid (b) were considered for the SRF injector and for the Max IV injector.

C. Optimization process

We optimized the amplitudes E_p and phases of the electric field in the photoinjector and accelerating cryomodule relative to the laser pulse arrival time to minimize bunch duration σ_t at the sample location. The focusing strength of the solenoids was adjusted to keep the bunch transverse size $\sigma_{x,y}$ on target below $100 \mu\text{m}$. For this purpose, the required magnetic flux did not exceed 50% of the field $B_{\max}$ listed in Table I.

III. RESULTS

Table II displays the simulation results for the Max IV photoinjector operating at a peak electric field on axis,

TABLE II. Beam parameters, E_p , and phase shifts for the Max IV photoinjector.

Φ FWHM	q	E	Gun E_p	φ_{Gun}	CM E_p	φ_{CM}	ϵ	σ_t
(μm)	(fC)	(MeV)	(MV/m)	($^\circ$)	(MV/m)	($^\circ$)	($\pi \times \text{nm} \times \text{rad}$)	(fs)
10	1	2	55	39	0.80	-100	3.2	1.7
10	1	5	55	5	5.1	-63.2	3.1	0.6
10	10	2	55	40	0.79	-99	6.2	2.0
10	10	5	55	5	5.1	-63.2	4.6	0.9
20	100	2	55	40	0.79	-99.4	21.9	4.1
25	100	5	55	5	5.2	-63.7	15.6	1.8

E_p , of 55 MV/m. The columns show the following parameters: laser spot size Φ , bunch charge q , beam energy E , peak electric field E_p in the gun and cryo-module, bunch projected emittance (ϵ), and σ_t at the sample location. Columns 5 and 7 show the phase shifts relative to the rf phase that result in the maximum beam energy gain in the gun and in both cavities, respectively. The phase shifts for both cavities are identical, even though the center of cavity 1 is located 6.842 m from the cathode, while the center of cavity 2 is positioned 8.189 m from the cathode. Figure 2 shows the evolution of bunch duration along the MeV-UED line for $E = 2$ MeV and $E = 5$ MeV. Figures 3 and 4 show evolution along the UED line of projected emittance and transverse beam size, respectively, for the beam energies 2 and 5 MeV, when bunches are generated in the Max IV photoinjector.

Table III presents the simulation results for the SRF photoinjector operating at a peak on-axis electric field E_p of 25 MV/m. As before, columns 5 and 7 show the corresponding phase shifts. For this study, all components

of the UED beamline—except for the injector—remained unchanged. Figure 5 shows the evolution of bunch duration along the MeV-UED line for $E = 2$ MeV and $E = 5$ MeV. Figures 6 and 7 show evolution along the UED line of projected emittance and transverse beam size, respectively, for the beam energies 2 and 5 MeV, when bunches are generated in the SRF photoinjector.

In the second part of the presented study, we focused on the impact of both the laser spot size and the transverse size of the electron bunch at the sample location on the bunch duration. The sample is located 12.5 m from the cathode.

We again considered bunch charges of 1, 10, and 100 fC, and beam energies of 2 and 5 MeV. Figure 8 shows results for the Max IV photoinjector, while Fig. 9 shows results for the SRF photoinjector.

As mentioned previously, the solenoids were set to maintain the electron bunches' transverse size $\sigma_{x,y}$ below 100 μm rms. For 100 fC, stronger focusing of the beam to approximately 50 μm increases the bunch duration by 5% due to the space-charge force. The minimum achievable transverse size for 100 fC was approximately 20 μm , but

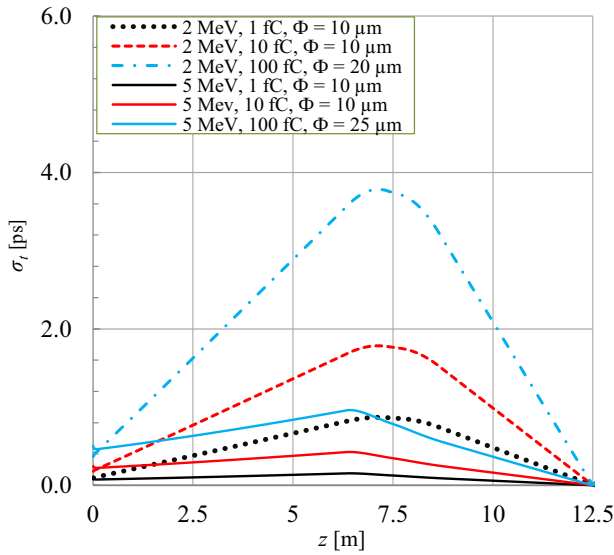


FIG. 2. Evolution of bunch duration along the MeV-UED line for $E = 2$ MeV and $E = 5$ MeV and 1, 10, and 100 fC charges. Bunches are generated in the Max IV photoinjector.

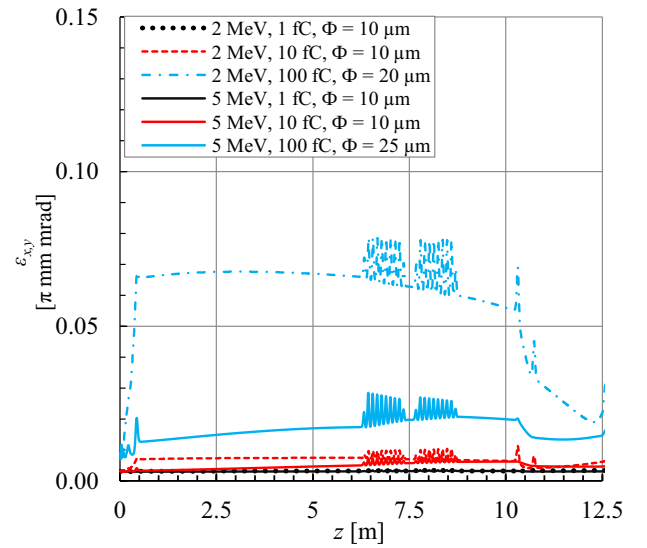


FIG. 3. Evolution of emittance along the MeV-UED line for $E = 2$ MeV and $E = 5$ MeV and 1, 10, and 100 fC charges. Bunches are generated in the Max IV photoinjector.

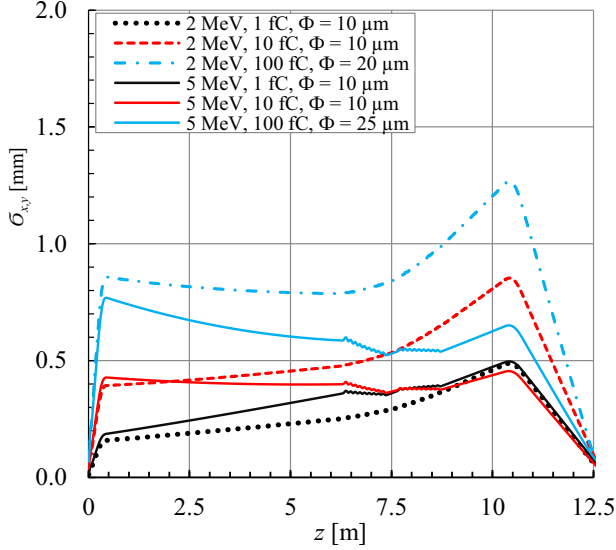


FIG. 4. Evolution of transverse beam size along the MeV-UED line for $E = 2$ MeV and $E = 5$ MeV and 1, 10, and 100 fC charges. Bunches are generated in the Max IV photoinjector.

the bunch duration nearly doubled. For 1 fC charge, focusing the beam to approximately $15\ \mu\text{m}$ increases bunch duration by 5%. The minimum achievable transverse size for a 1 fC was below $4\ \mu\text{m}$ for 2 MeV and below $1.5\ \mu\text{m}$ for 5 MeV, but again, the bunch duration almost doubled. This phenomenon arises from the space-charge force, which becomes significantly stronger for bunches with higher charge.

IV. TIME JITTER CONSIDERATIONS

Timing jitter is one of the key factors limiting the achievement of high temporal resolution in ultrafast electron diffraction setups. In our study, we analyzed the influence of timing jitter using the semianalytical approach introduced in [18]. This method enables rapid estimation of arrival-time jitter arising from rf phase and amplitude instabilities, while also allowing the minimization of bunch duration. Timing jitter can be optimized by carefully selecting the amplitudes and phases of the rf fields within the accelerating cavities.

Our findings show that the optimal rf configuration depends strongly on the level of rf stability. For relatively large rf instabilities—such as a 0.01% relative amplitude variation and a 0.05° phase variation (as assumed in Ref. [8])—the best performance is achieved when the rf gun operates near the on-crest phase (configuration 1). In this configuration, by adjusting the phases and amplitudes in the subsequent accelerating structures to minimize the bunch duration, the time-of-flight (TOF) jitter can be reduced to approximately 100 fs at an electron beam energy of 2 MeV. This result, derived using the semi-analytical model from Ref. [18], is consistent with the values reported in Ref. [8] under similar conditions. Under lower-jitter conditions, however, a configuration studied in this work—where the rf gun is tuned close to the phase that minimizes its own time of flight, referred to as configuration 2—outperforms configuration 1. For brevity, we present results for configuration 2 corresponding to the parameters in the first row of Table III, i.e., for an electron beam energy of 2 MeV. In this regime, both the bunch duration and TOF jitter improve significantly. We have verified that under high-jitter conditions (0.01% amplitude and 0.05° phase variation), configuration 2 performs worse than configuration 1, yielding a TOF jitter of about 140 fs. However, under improved rf stability (0.01% amplitude variation and 0.01° phase variation), configuration 2 clearly outperforms configuration 1, achieving a TOF jitter of only 30 fs compared with 80 fs for configuration 1. These results demonstrate that the optimal configuration for UED depends critically on the rf stability of the system.

If the rf amplitude and phase jitters are measured on a shot-by-shot basis, this information can be used to calculate the actual timing jitter for each pulse, enabling data postcorrection [18]. To reduce the corrected TOF jitter below 10 fs using configuration 2 at 2 MeV electron beam energy, the rf measurement accuracy must exceed 0.003% for amplitude and 0.003° for phase. At the same rf measurement accuracy, the configuration used for a 5 MeV electron beam (second row of Table III) is expected to yield a corrected jitter below 5 fs. Current advances in low-level rf (LLRF) technology, particularly

Table III. Beam parameters, E_p , and phase shifts for the SRF photoinjector.

Φ FWHM	q	E	Gun E_p	φ_{Gun}	CM E_p	φ_{CM}	ε	σ_t
(μm)	(fC)	(MeV)	(MV/m)	($^\circ$)	(MV/m)	($^\circ$)	($\pi \times \text{nm} \times \text{rad}$)	(fs)
10	1	2	25	40.0	0.78	−101.7	3.0	1.5
10	1	5	25	5.0	5.0	−62.9	3.1	0.6
15	10	2	25	40.0	0.80	−101.9	8.8	2.2
20	10	5	25	5.0	5.0	−63.1	6.9	1.2
28	100	2	25	40.5	0.77	−101.8	19.3	4.6
50	100	5	25	0.0	4.9	−62.9	22.6	2.1

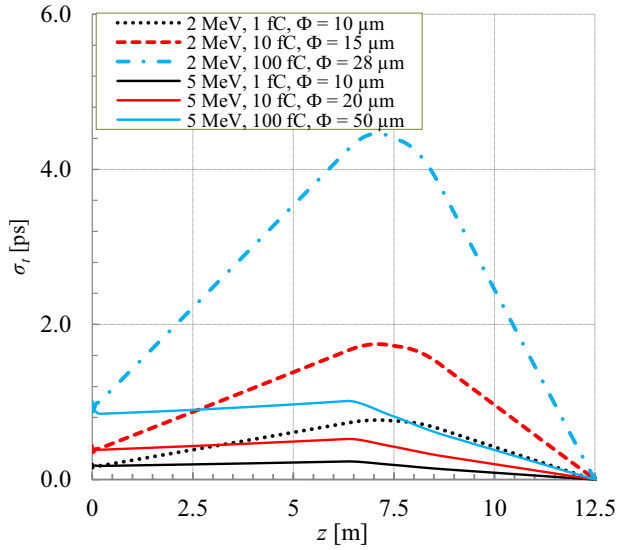


FIG. 5. Evolution of bunch duration along the MeV-UED line for $E = 2$ MeV and $E = 5$ MeV, and 1, 10, and 100 fC charges. Bunches are generated in the SRF photoinjector.

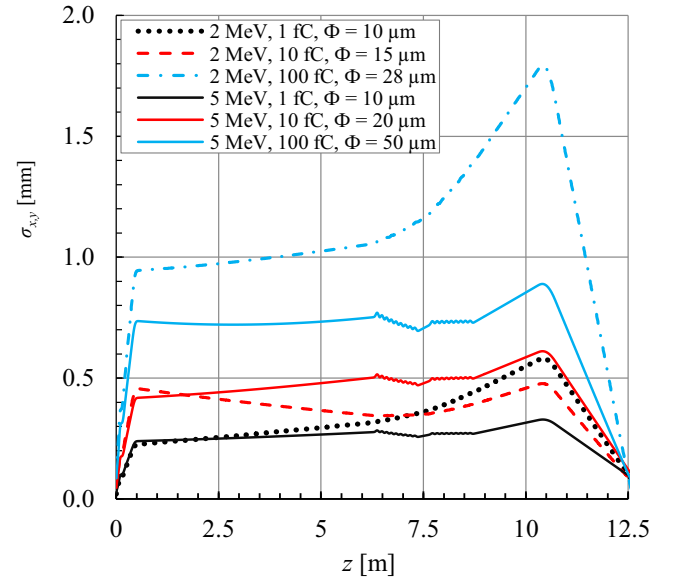


FIG. 7. Evolution of transverse beam size along the MeV-UED line for $E = 2$ MeV and $E = 5$ MeV and 1, 10, and 100 fC charges. Bunches are generated in the SRF photoinjector.

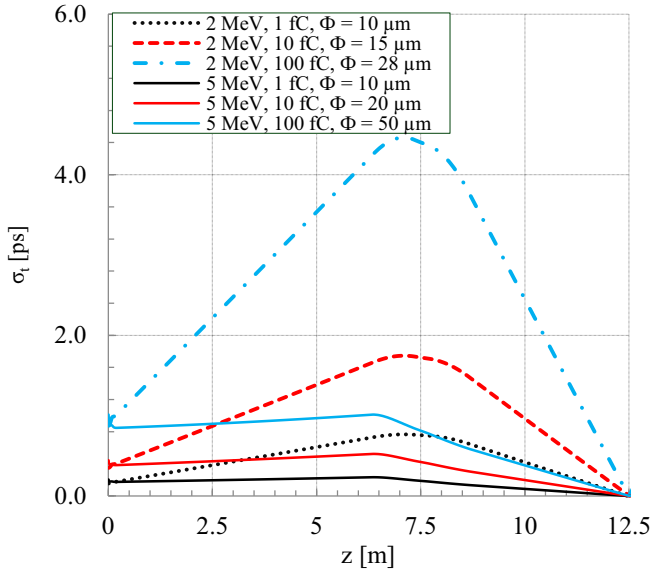


FIG. 6. Evolution of emittance along the MeV-UED line for $E = 2$ MeV and $E = 5$ MeV and 1, 10, and 100 fC charges. Bunches are generated in the SRF photoinjector.

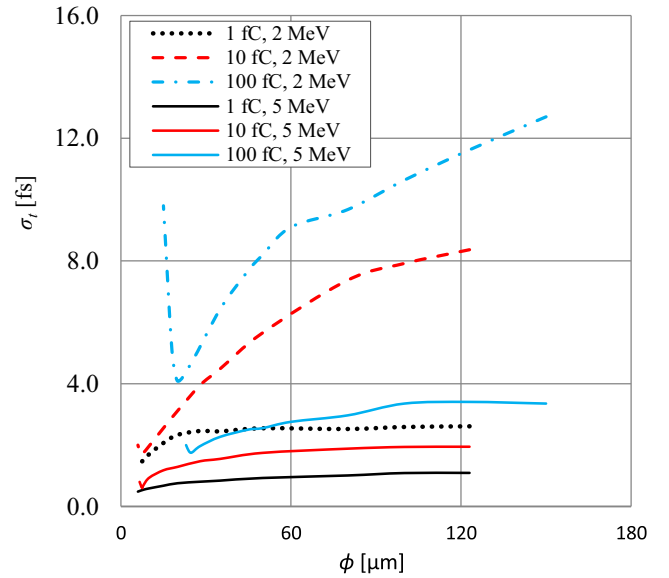


FIG. 8. Bunch duration σ_t at the sample location versus laser spot size Φ at the Max IV injector cathode for $E = 2$ MeV and $E = 5$ MeV.

for superconducting cavities, show great promise in achieving this level of precision [19].

V. DISCUSSION

The study showed that for a charge range of 1–100 fC, and beam energies of 2 and 5 MeV with proper setting of the following parameters: (i) gradients and phases in the

injector and cryomodule; (ii) amplitudes of magnetic flux in both solenoids; and (iii) diameter of the laser spot on the cathode Φ , the ballistic compression led to a duration of bunches $\sigma_t < 5$ fs for all considered cases. By adjusting the second solenoid (d), the transverse size of bunches $\sigma_{x,y}$ at the sample location can be kept below 100 μm . For significantly smaller $\sigma_{x,y}$ at the sample location, it should be noted that the bunch duration increases as a result of the space-charge force.

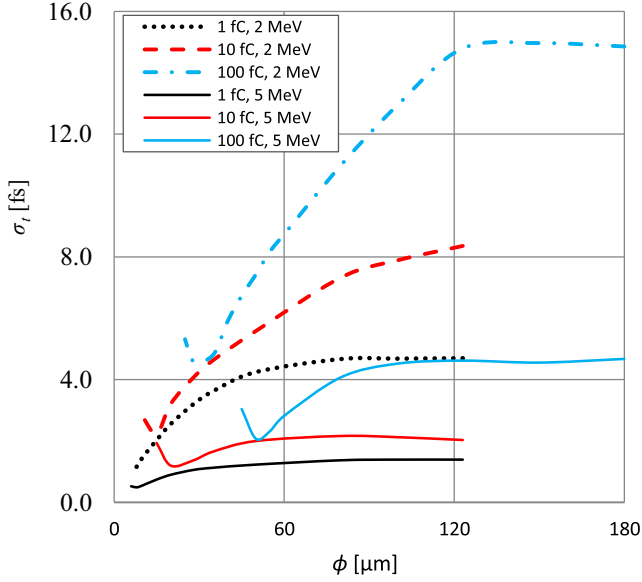


FIG. 9. Bunch duration σ_t at the sample location versus laser spot size Φ at the SRF injector cathode for $E = 2$ MeV and $E = 5$ MeV.

Next, the study of σ_t versus Φ showed that, for 10 and 100 fC emitted from either injector, the bunch duration increases for $\Phi < \Phi_{\min}$, where $\Phi_{\min}$ indicates spot size for the shortest duration at location of the tested sample (see Table IV).

This phenomenon is due to the space-charge force. It occurs for the SRF photoinjector, which was assumed to operate at $E_p = 25$ MV/m, for larger $\Phi_{\min}$ values than those calculated for the Max IV injector, which was assumed to operate at 55 MV/m. We intentionally set the operating gradients for both injectors well below the demonstrated gradients to minimize the likelihood of dark current generation in the facility.

For 100 fC and $E = 2$ MeV, in the case of Max IV photoinjector, σ_t increases with Φ for $\Phi > \Phi_{\min}$. For the SRF photoinjector, at 100 fC charge and $E = 2$ MeV, σ_t is larger than for the Max IV injector and reaches a plateau when $\Phi > 120$ μm . In the case of 100 fC and $E = 5$ MeV, for both photoinjectors σ_t saturates when $\Phi > 100$ μm . For 1 fC and both beam energies, σ_t stays below 5 fs for either of the injectors.

TABLE IV. $\Phi_{\min}$ FWHM values for both injectors.

Q	E	Max IV $\Phi_{\min}$	SRF $\Phi_{\min}$
(fC)	(MeV)	(μm)	(μm)
10	2	7	15
10	5	7.5	20
100	2	20	28
100	5	25	50

VI. SUMMARY AND PROSPECTS

This study demonstrates that the MeV-UED beamline, comprising electron photoinjectors and a superconducting HZDR/RI-type cryomodule, can deliver electron bunches with durations below 5 fs for charges of 1–100 fC and beam energies of 2 and 5 MeV.

We observed that the minimal bunch duration, σ_t , generally decreases as the laser spot size, Φ , at the injector's photocathode decreases. However, for higher charges emitted from either injector, σ_t begins to increase below a certain threshold, $\Phi_{\min}$, due to the space-charge effect. Furthermore, tightly focusing the electron bunch at the sample location increases its duration even further because of the same effect.

The planned MeV-UED facility at NCBJ can be compared with state-of-the-art installations such as SLAC [20], KAERI [21], Tsinghua University [22], Shanghai Jiao Tong University [23], REGAE (DESY) [24], and the upcoming SEALab (HZB) [25]. Unlike the warm rf guns used at most existing facilities, both NCBJ and SEALab will employ superconducting technology in cw mode, enabling repetition rates of up to 1 MHz. While existing and planned facilities have, or aim to achieve, comparable bunch durations and beam emittances, their low repetition rates limit signal-to-noise ratios and hinder studies of weakly scattering systems. In contrast, the cw operation at NCBJ will enable the investigation of such samples while also supporting very low charge bunches—from femtocoulomb to subfemtocoulomb levels—which reduces space-charge effects, preserves beam quality, and generates ultrashort, few-femtosecond pulses. This capability opens entirely new experimental opportunities for ultrafast electron diffraction.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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