

FIRST CONCEPTUAL DESIGN STUDIES OF AN ELECTRON SOURCE FOR ULTRAFAST ELECTRON DIFFRACTION AT DELTA*

D. Krieg[†], S. Khan, Center for Synchrotron Radiation, TU Dortmund University, Dortmund, Germany
K. Sokolowski-Tinten, University Duisburg-Essen, Duisburg, Germany

Abstract

Ultrafast electron diffraction (UED) is a technique to study the structural dynamics of matter, combining diffraction of electrons with sub-angstrom De-Broglie wavelength with femtosecond time resolution. The method is complementary to X-ray scattering at free-electron lasers. UED pump-probe experiments require ultrashort laser pulses to pump a sample, electron bunches with small emittance and ultrashort length to analyze the state of the sample by diffraction, as well as excellent control of the delay between them. While most UED systems are based on electrostatic electron sources in the keV regime, electrons accelerated to a few MeV in a radiofrequency photocathode gun offer significant advantages regarding emittance and bunch length due to the reduction of space charge effects. Furthermore, the longer mean free path of MeV electrons allows for thicker samples and hence a broader range of possible materials. In this paper, a first conceptual design and simulation results for a university-based UED facility with ultrashort and low-emittance MeV electron bunches are presented.

INTRODUCTION

Ultrafast electron diffraction (UED) is a technique to explore structural dynamics of matter e.g. as a pump-probe with an optical pump and an electron bunch as probe. The technique has to satisfy the relevant spatial (sub-1 Å) and temporal (sub-100 fs) resolution. The scattering cross section for electrons is 10^4 to 10^6 times higher than for X-rays so that a small number of electrons is sufficient to achieve results comparable to X-ray scattering [1]. However, a very high electron beam quality is required. The study of, e.g., proteins requires a coherence length of 30 nm, which translates into a beam divergence of $12.5 \mu\text{rad}$ at a bunch radius of 0.2 mm [2]. Moreover, short and reproducible bunch lengths down to some tens of fs are required. In most cases, UED is performed using keV DC electron sources. They have been improved over years and produced scientific results. The usage of MeV electrons, i.e., by employing radiofrequency (rf) photoinjectors has several advantages [1].

1. The higher acceleration gradient allows to rapidly accelerate the electrons to relativistic energies. This suppresses space charge effects, because both, the transverse and the longitudinal space charge force acting on a particle in the bunch, scale as $1/\gamma^2$ with the Lorentz factor γ [3]. The generation of brighter electron beams with shorter bunch length is possible.

2. MeV electrons move nearly with the velocity of light so that there is no velocity mismatch with the optical pump pulse.
3. The elastic and inelastic mean free path lengths are larger so that the use of thicker samples is possible.

Recently, a design study for a university-based UED facility providing high-quality electron bunches was initiated at the Center for Synchrotron Radiation of the TU Dortmund University which also operates the 1.5-GeV synchrotron light source DELTA. In this paper, first simulation results are presented.

BASIC DESIGN

In Fig. 1, two options for a conceptual design of an UED setup are shown. In both cases, the electrons are emitted via a laser pulse hitting the photocathode, which is placed inside of a 1.5-cell standing-wave cavity. For a cavity with a radiofrequency of 3 GHz, for example, the accelerating gradient in the gun cavity is around 100 MV/m which rapidly accelerates the electrons to relativistic energies. The subsequent solenoid compensates the transverse defocussing of the cavity [4,5]. The electron source is followed by the target chamber, a detection system and the beam dump. Using the photocathode laser also to excite the sample would provide a natural synchronization for pump-probe measurements. In the second option of Fig.1, a bunching cavity is used to provide additional longitudinal focusing. It is operated off-crest and imprints an energy chirp onto the electron distribution

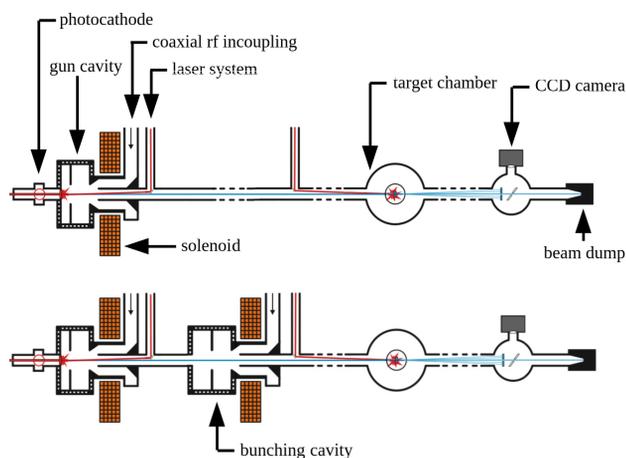


Figure 1: UED setup without (top) and with a bunching cavity (bottom) .

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[†] daniel.krieg@tu-dortmund.de

such that particles at the tail of the bunch gain a higher velocity than those at head. The use of a bunching cavity has two main advantages:

1. The additional radiofrequency (rf) amplitude and phase provide more flexibility in adjusting the longitudinal focus.
2. The bunching cavity allows to linearize the longitudinal phase space distribution without harmonic cavities [6].

The main disadvantage of the usage of a bunching cavity is that a second rf transmitter or a circulator is needed to avoid coupling between the cavities. In addition, the bunching cavity has to be synchronized to the laser and the gun cavity precisely.

MAIN LIMITATIONS

There are two main limitations for ultrashort high-brightness electron bunches: The Coulomb repulsion of the electrons enlarges the bunch in all dimensions in a nonlinear way. The transverse space charge field scales as $E_r \propto r/R^2$ with the radial position r inside the bunch and the bunch radius R . In longitudinal direction, it scales as $E_z \propto z/L$ with the longitudinal position z in the bunch and the bunch length L [3, 7]. Secondly, the curvature of the accelerating field is translated into nonlinearities in the longitudinal phase space. The accelerating field [7]

$$E_z(z, t) = E_0 \sin(\omega t + \varphi) \cos(k_z z), \quad (1)$$

depends on the time t at which an electron is emitted. Moreover, there is a nonlinearity of the longitudinal compression process itself. A relative shift of the electrons in a drift space is given by the velocity difference within the bunch which is based on the energy chirp induced by the bunching cavity. The correlation between energy and velocity β is given by $\gamma = 1/\sqrt{1 - \beta^2}$. As a consequence, for any imprinted energy chirp that does not yield a linear velocity spread, a curvature and higher-order distortions are generated in the longitudinal phase-space distribution of the electrons. [6, 8].

Table 1: Main Simulation Parameters

bunch charge	100 fC
accelerating gradient	100 MV/m
rms laser radius at cathode	10 μm
rms pulse length of laser	100 fs
initial kinetic energy	0.27 eV
work function of cathode material	3.5 eV
laser photon energy	4.66 eV
frequency gun cavity	3 GHz
# of cells gun cavity	1.5
distance from gun to focus	5 m
transverse bunch radius at focus	0.5 μm
number of macro particles	1000

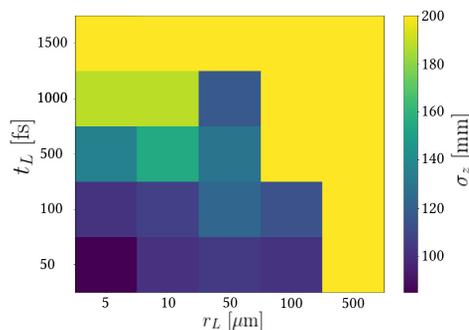


Figure 2: Minimum rms bunch length σ_z color-coded as function of the laser spot size r_L at the cathode and the laser pulse length t_L .

SIMULATION STUDIES

First simulation studies with ASTRA [9] including space charge effects were performed. The ultimate goal of the simulation studies is to find a UED design, satisfying temporal and spatial requirements. For this purpose, the design without bunching cavity is chosen because the observable space charge effects and nonlinearities of the phase space should be similar to those including a bunching cavity. At first, the influence of the starting emittance at the cathode on the rms length σ_z of the electron bunch was investigated. The parameters used for this simulation can be found in Table 1. The electron bunch was longitudinally focused at $z_f = 5.0$ m. Figure 2 shows a color-coded representation of σ_z at the position z_f of the focus under variation of the laser spot radius r_L at the cathode and the laser pulse length t_L . With the solenoid parameters, both, the transverse divergence was minimized at z_f and the bunch radius was adjusted to 0.5 mm at z_f . With a smaller laser spot radius at the cathode or a shorter laser pulse length, the starting emittance is smaller and shorter bunch lengths σ_z in the focus are possible. A bunch charge of $Q = 100$ fC was chosen because this is typically required for UED at MeV energies [1, 8].

Space Charge Effects

The smallest bunch length σ_z at the longitudinal focus is a measure for the influence of the space charge effects. Figure 3 shows σ_z under variation of the accelerating gradient E_0 and the bunch charge Q . The bunch length has a minimum

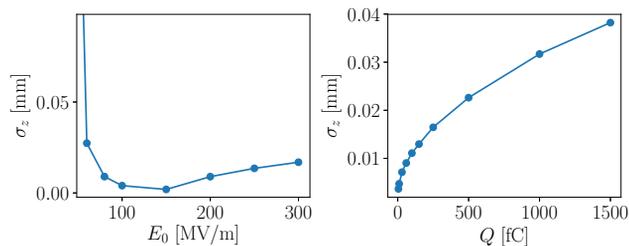


Figure 3: Left: Rms bunch length σ_z in longitudinal focus with different amplitudes E_0 of accelerating gradients in the gun cavity. Right: σ_z as function of bunch charge Q .

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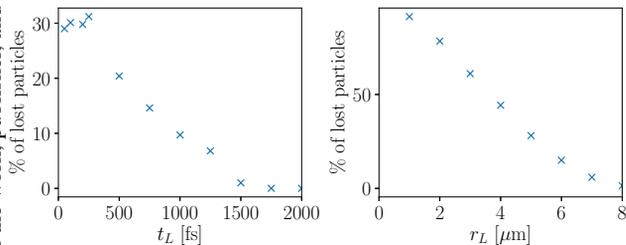


Figure 4: Percentage of lost particles as function of the laser pulse length t_L and the laser spot radius r_L .

between 100 MV/m and 150 MV/m. The maximum available acceleration gradient for a gun cavity with a frequency of $f = 3$ GHz is $E_{0,\text{max}} \approx 110$ MV/m. With increasing bunch charge Q , the bunch length increases as expected. A simulation with a gun cavity at a frequency of $f = 1.3$ GHz and an acceleration gradient of $E_0 = 60$ MV/m [10] shows a loss of particles caused by space charge effects. In Fig. 4, the percentage of lost particles due to space charge effects as a function of the laser spot radius at the cathode r_L and the laser pulse length t_L is shown. A lower electron density at the cathode, larger r_L and/or t_L causes a weaker Coulomb repulsion and hence less particles are lost.

Nonlinearities

To investigate the rf-induced nonlinearities in the longitudinal phase space, simulations with gun cavity frequencies of 1.3 GHz, 3.0 GHz and 6.0 GHz were performed with a laser pulse length of $t_L = 100$ fs and a laser spot radius of $r_L = 10$ μm . The choice of these values ensures that no particles are lost in the $f = 1.3$ GHz setting (Fig. 4). Figure 5 shows the evolution of σ_z along the electron path as well as the longitudinal phase-space distribution at the longitudinal focus z_f . The smallest σ_z is limited by the nonlinearities as well as space charge effects. The nonlinearities increase with the frequency f , because for a given bunch length a wider range of the sinusoidal curvature of the accelerating field is translated into the longitudinal phase-space distribution.

CONCLUSION AND OUTLOOK

Space charge effects and nonlinearities are limiting factors for a high-quality electron beam. To suppress the space charge effects, a high acceleration gradient or a low bunch charge is required. A small starting emittance is important to generate short bunches but on the other hand it boosts space charge effects because of the high electron density at the cathode. Rf-induced nonlinearities can be suppressed by using lower rf frequencies. Typically, the acceleration gradient is not high enough to suppress space charge effects efficiently for the required bunch charge. This can be seen by the particle losses in the case of the 1.3 GHz gun cavity. Another way of reducing the nonlinearities is to use a harmonic cavity [11] or a stretcher mode, a linearization scheme without harmonic cavities [6]. In this scheme, the induced energy spread induced by the gun phase settings leads to a

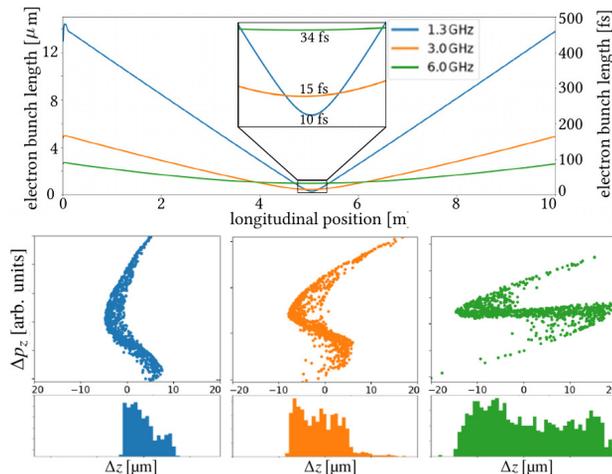


Figure 5: Top: Electron bunch length at the longitudinal position of the electron source for the three simulation settings. Bottom: Longitudinal phase spaces at the longitudinal focus of the three simulation settings.

controlled expansion of the electron bunch in the drift space. As a consequence, the curvature in phase-space and higher-order distortions change as well. The subsequent bunching cavity is used for linearizing and can be operated at the same frequency as the gun cavity. The field of the bunching cavity effectively acts like a higher-harmonic structure, because the associated field curvature is larger than the expanded bunch nonlinearities [6]. The simulation results also show that bunch lengths < 100 fs and the divergence ≈ 10 μrad required for the spatial resolution < 1 \AA are reachable. As for the rf frequency, 1.3 GHz will be not the best choice. The simulation shows that the possible acceleration gradients are not high enough to efficiently suppress the space charge effects. On the other hand, 6 GHz would lead to a strong influence of the nonlinearities. As a result of the present studies, the first choice for the rf frequency is $f = 3$ GHz.

It has to be studied whether a design with or without a bunching cavity provides the best beam quality. For this purpose, the solenoid optics has to be worked out as well as the laser and rf incoupling.

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