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PROSPECTS OF ULTRAFAST ELECTRON DIFFRACTION EXPERIMENTS AT SEALab

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Abstract

Ultrafast Electron Diffraction (UED) is a pump-probe experimental technique that aims to image the structural changes that happen in a target structure due to photo-excitation. Development of MeV UED capabilities is one of the main objectives at Sealab, a superconducting RF accelerator facility being commissioned in Helmholtz-Zentrum Berlin. In order to perform UED experiments, the optimization of temporal resolution is of the utmost importance. The composition of the SRF Photoinjector, currently the main beam-line in Sealab, offers superb flexibility to manipulate the longitudinal phase-space of the electron bunch. At the same time, the CW operation of the accelerator provides an enhanced beam stability compared to warm guns, together with a MHz repetition rate. This work aims to show the capacity of the SRF Photoinjector in Sealab to reach the required temporal resolution and explain the development and current status of the necessary tools to perform UED experiments at the facility.

INTRODUCTION

Over the last decade, cost-effective and compact Ultrafast Electron Diffraction (UED) machines have opened an era for examining an ultrafast structural dynamics associated with the diffraction of phase transformations and making and breaking of bonds in solids, chemical reactions, and rapid biological processes which was only allowed for the much larger Free Electron Lasers (FELs). Recent progress on semiconductor-based photocathodes have pushed thermal emittances down to few nanometer-radian at a femtocoulomb bunch charge, resulting in MeV-class electrons produced by a gun having the transverse coherency close to the hard X-rays. The strong scattering power of electrons enables observation of atomic and molecular structures at low intensity. The MeV-class beam energy increases penetration depth and accomplishes sufficient bunch charges at a short bunch length. These features enable the fine scanning of the structure at different time steps attained by adjusting the time-delay between pump and probe pulses. The remaining challenge of MeV-class UED accelerators is the generation of extremely short bunches with consummately reliable stability in terms of beam arrival time for achieving a high temporal resolution as well as sufficient lateral coherency. The SRF Photoinjector in Sealab is well suited for this purpose.

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SEALab

Superconducting Electron Accelerator Laboratory (Sealab) in Helmholtz-Zentrum Berlin is a test bench for beam dynamics, control and instrumentation R&D of high average current, ultrashort and high brightness beams. The main beam-line within the Sealab facility is a SRF Photoinjector. Offering user dedicated UED capabilities is among the goals of Sealab. A simplified sketch of the beam-line can be seen in Fig. 1. The laser system provides green light between 510 nm and 540 nm. The repetition rate of the laser system can reach 1.3 GHz. The laser spot size at the photocathode is limited in the lower side to 0.5 mm rms radius top-hat distribution. It has a minimum pulse length of 1.0 ps and a Gaussian longitudinal shape. The photocathode is located at the back-wall of a superconducting L-band (1.3 GHz) electron gun. Three more L-band superconducting booster cavities are located between the gun and the target station. All cavities operate in continuous wave (CW) mode.

Since the injectors of energy recovery linear accelerators (ERLs) produce intense electron beams of superior quality in 6-D phase space with an equivalent layout to the SRF Photoinjector, the approach presented here offers special scientific opportunities for these facilities. Given the capacity of superconducting injectors to operate with one bunch per RF cycle, this open the door for MHz repetition rate UED experiments, greatly increasing the signal to noise ratio.

METHODS

Different tasks are currently being undertaken with the goal of enabling high resolution UED capabilities in the SRF Photoinjector and develop the necessary tools for user operation. Amongst them are the study of time resolution optimization [1], the design of beam diagnostics systems for low intensity beams and short bunches [2], the development of a surrogate model of the SRF Photoinjector based on neural networks and the preparation of a proof of concept static diffraction experiment.

Time Resolution Optimization

The time resolution R_t in a UED experiment defines the capability of discerning minimum temporal extension of the structural dynamics. This quantity can be expressed by a square root of the sum of the quadrature of the different contributions,

$$R_t^2 = \sigma_{pump}^2 + \sigma_{probe}^2 + \tau_{jitter}^2 + \tau_{vm}^2,$$

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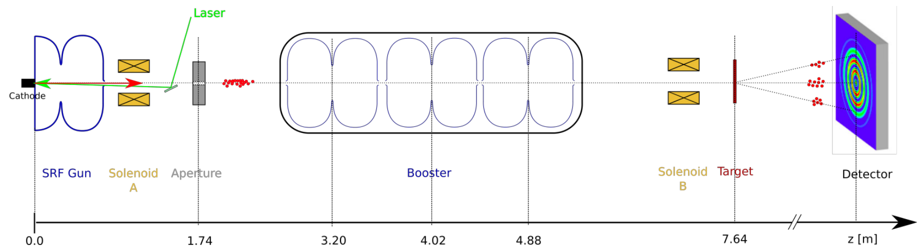

Figure 1: Sketch of the SRF Photoinjector beam-line with UED related components.

where σ_{pump} and σ_{probe} stand for the rms length of the laser and electron pulses at a sample, respectively, τ_{jitter} refers to the fluctuation in elapsed time between the arrival of two pulses, and τ_{vm} represents the velocity mismatch. MeV electron beam energies reduce this last contribution to the point of being neglectable compared to lower energy electron beams. For obtaining a bunch length of sub-100 fs at a bunch charge of 100 fC, new schemes have been devised [3]. The fluctuation of elapsed time between pump and probe pulses, the so-called timing jitter τ_{jitter}, however, overwhelms the temporal distribution of electrons in a bunch, so it limits the temporal resolution of the whole system. Therefore, in modern UED facilities, the challenge tackled is to achieve an optimum temporal resolution by compromising both contributions as defined by Renkai Li et al. [4]. In that case, the phase of radio-frequency (RF) fields in a gun is adjusted to a slight off-crest value for obtaining the minimum bunch length. However, the time resolution in this approach is limited due to the enhancement of the initial RF to laser jitter by setting the off-crest phase. In addition, an ultrashort laser pulse is required at the cathode. Here, we use the multiple cavities available downstream the gun in the SRF Photoinjector to ameliorate the temporal resolution. This allows to free the gun cavity from the burden of a bunch compression and choose the best emission phase for suppressing the timing mismatch between the laser and RF fields. In addition, multiple cavities permit the manipulation of electron distribution in longitudinal phase-space using a linearization method based on the stretcher mode [3], which can reduce the minimum bunch length at the target by compensating for the nonlinear distortion caused by space charge forces. The working points of the RF cavities that lead to minimum values of the ToF jitter and bunch length are not the same, hence a compromise has to be found. This trade-off has been studied for different number of cavities in the beam-line [1]. The pareto-fronts which represent the set of non-dominated solutions, where each objective are considered as equally good are estimated and shown in Fig. 2 together with the minimum achievable time resolution shown with an arc with $R_{min} = \sqrt{\sigma_{probe}^2 + \tau_{jitter}^2}$ for each case. The trade-off between compression and jitter can be observed from the result. It is clear that the use of multiple cavities in the beam-line increases the maximum achievable time resolution. The highest value achievable in the SRF Photoinjector, while keeping an lateral coherence length of at least 3 nm, is limited to 103 fs by the field instabilities in the RF cavities.

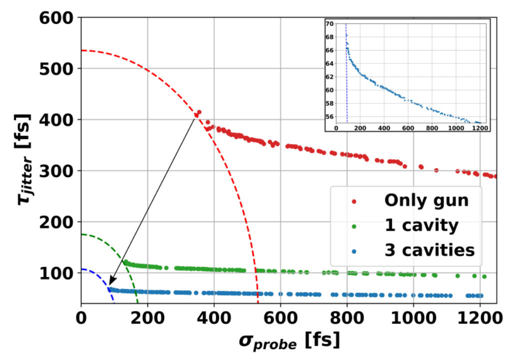

Figure 2: Compromised solutions calculated by a multi-objective genetic algorithm [5] for the optimization of the time resolution in the SRF Photoinjector. The red dots represent the pareto-dominant solutions for the beamline with only gun, the green dots represent the solutions for a single additional cavity and the blue dots represent the solutions for three additional cavities. The insert plot shows the zoom of the latest. The dashed lines represent the minima for each chase. The optimization constrains are that the initial laser pulse length at the cathode has to be longer than 1 ps, the initial rms laser spot size larger than 0.5 mm and that the electron bunch at the target must have a charge of at least 50 fC.

UED Surrogate Model

In order to enhance the operation capabilities of the UED experiments in Sealab a surrogate model based on neural network has been developed. The model is able to imitate the behaviour of the machine faster and without the need to simulate. An sketch of the model with some input and the output parameters is shown in Fig. 3.

The model containing 13 inputs and 5 outputs is built by using a neural network based on previous work by D. Meier et al. [6], with the 4 hidden layers having 2022, 447, 100 and 22 neurons respectively. The training dataset contains $5{\times}10^5$ data points simulated using Astra by initializing the input parameters randomly inside an initial parameter space suitable for UED. The regression results are shown in Fig. 4 and show that the model is able to accurately train and predict the output of the system. The time needed to track $20{\times}10^3$

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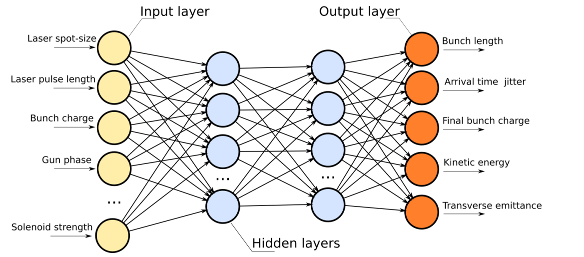

Figure 3: Neural network composition for training the SRF Photoinjector surrogate model.

particles from the cathode to the target including space-charge fields is in the 10 minute range, while a call to the surrogate model under the same conditions is performed in ms time scales once it has been trained. The next step planned for the near future is to invert the model in order to give a quick response to any output parameter request from the UED users in Sealab.

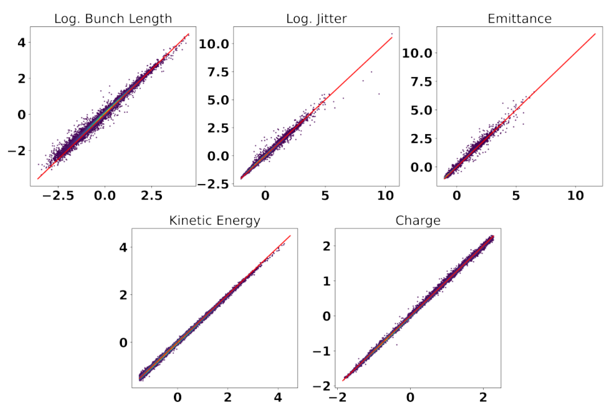

Figure 4: Outputs from the surrogate model after training (y_{model}, Y axis) are plotted against the output values from simulations ($y_{simulation}$, X axis) for the same input parameters. The input and output values have been scaled before training in order to improve results. For two of the outputs (bunch length and ToF jitter) a logarithm has also been applied in order to reduce the several magnitude order range. In a perfect surrogate model all points would fall in the red lines given by $y_{model} = y_{simulation}$ for every output.

Diagnostics for UED

The measurement of beam properties under extreme beam requirements expected for UED and other similar applications such as plasma accelerators require original diagnostics solutions. In this direction, a beam size monitor with μm resolution has been designed and experimentally tested. An sketch of the system can be seen in Fig. 5. This monitor relies the interferometric pattern produced by using a suitable double slit for the coherent synchrotron radiation emitted by very short bunches. The nature of the coherent radiation ($\propto N^2$) makes this method suitable for low intensity beams. The results have been published [2]. In addition, a transverse deflector cavity has also been installed in the beam-line for bunch length measurements [7]. Work is ongoing to develop a arrival time detector for low intensity beams based on a RF cavity.

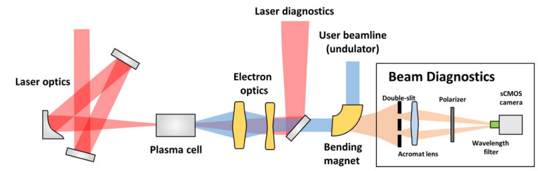

Figure 5: Schematic layout of the interferometry beam size monitor (IBSM) for a plasma-wakefield accelerator.

Preparation of Static Diffraction Experiment

In order to characterize the quality of the beam for UED experiments and test new emittance measurement techniques using TEM grids [8] a static diffraction experiment is planned for the next months. The beam-line elements required for this experiment have been designed and are already built. A picture of the sample holder is shown in Fig. 6. Appropriate samples for UED have been produced in collaboration with Fritz Haber Institute and are going to be tested by our partners in Humboldt Universität zu Berlin before the installation in the beam-line.

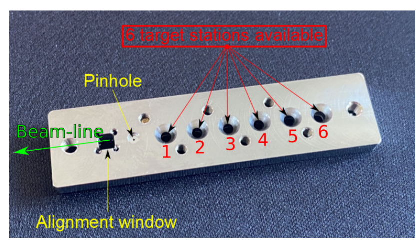

Figure 6: Picture of the sample holder for static diffraction experiments.

CONCLUSIONS

The tools to enable MeV UED in Sealab are being steadily developed. A method to increase time resolution of UED experiments to the maximum in the SRF Photoinjector has been developed and simulations show that appropriate beam characteristics can be achieved for diffraction experiments. This will soon be tested experimentally. Neural networks have been successfully applied to build a surrogate model that can mimic the behaviour of the SRF Photoinjector. The model will be inverted to deliver a quick tailored response to any user request in the future. Finally, diagnostics tools for extreme beam conditions have been studied and a spot size monitor with μm resolution has been designed and successfully tested.

REFERENCES

[1] Alberdi-Esuain, B. et al.,"Novel approach to push the limit of temporal resolution in ultrafast electron diffraction accelerators". *Submitted to Sci. Rep.* (June 2022).

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[2] J.G. Hwang, *et al.*, "Monitoring the size of low-intensity beams at plasma-wakefield accelerators using high-resolution inter-ferometry", *Commun. Phys., vol.* 4, p. 214, 2021.

[3] B. Zeitler, *et al.*, "Linearization of the longitudinal phase space without higher harmonic field", *Phys. Rev. Accel. Beams, vol.* 18, p. 120102, 2015.

[4] R.K. Li, *et al.*, "Temporal resolution of MeV ultrafast electron diffraction based on a photocathode RF gun", *Nucl. Instrum. Methods Phys. Res., Sect. A, vol.* 605, p. 243, 2009.

[5] E. Zitzler and L. Thiele, "Multiobjective evolutionary algo-rithms: a comparative case study and the strength Pareto approach", IEEE Trans. Evol. Comput. vol. 3, p. 257, 1999.

[6] D. Meier, *et al.*, "Reconstruction of offsets of an electron gun using deep learning and an optimization algorithm". *Proc. SPIE*, 11493, 2021.

[7] G. Kourfakas, *et al.*, "Transverse deflecting cavity for longitu-dinal beam diagnostics at bERLinPro", *Proc. 29th Int. Linear Accelerator Conf. (LINAC'18)*, Beijing, China 2018.

[8] D. Marx, *et al.*, "Single-shot reconstruction of core 4D phase space of high-brightness electron beams using metal grids", *Phys. Rev. Accel. Beams,* vol. 21, p.102802, 2018.