EuPRAXIA Doctoral Network

Unlocking atomic motion: Dielectric THz-driven Accelerators for Ultrafast Electron Diffraction

Andrés Leiva Genre

University of Pécs

Szentágothai Research Center

Supervisor: Dr. Szabolcs Turnár

Prof. Dr. Gábor Almási

15 July 2025

UK Research and Innovation

Outline

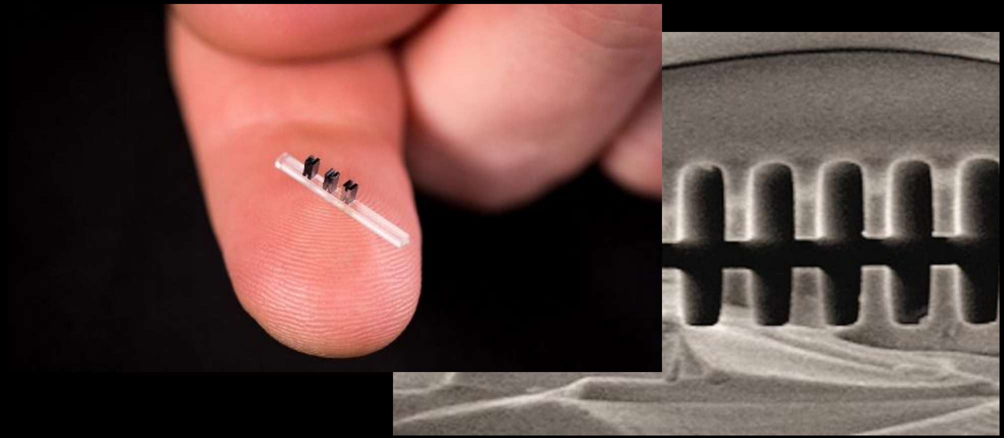
Doctoral Network

- **Quick overview of Dielectric Laser-driven Accelerators (DLAs)**
- **Ultrafast Electron Diffraction (UED)**
  - ✓ Main ideas and figure of merits
  - ✓ THz pulses: Setups & their Benefits in UED
  - ✓ Dielectric THz-driven Accelerators (DTAs)
  - ✓ Fundamental Science Drivers for UED

MOTIVATION

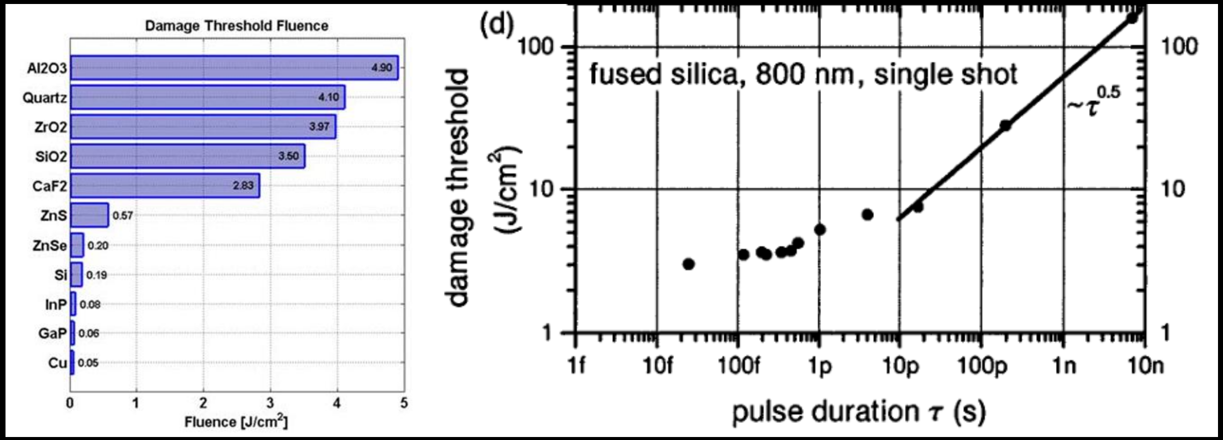
EuPRAXIA Doctoral Network

SIZE



Accelerating dielectric microstructures. Images from *achip.standford.edu*.

POWER LIMITATION



Left: Ken Soong et. al.; Laser damage threshold measurements of optical materials for direct laser accelerators. *AIP Conf. Proc.* 21 December 2012; 1507 (1): 511–515

Right: Tien, An-Chun, et al. "Short-pulse laser damage in transparent materials as a function of pulse duration." *Physical Review Letters* 82.19 (1999): 3883.

DTA: ACCELERATION CONCEPT

Acceleration is attained by the **near-fields** provided by the dielectric structure.

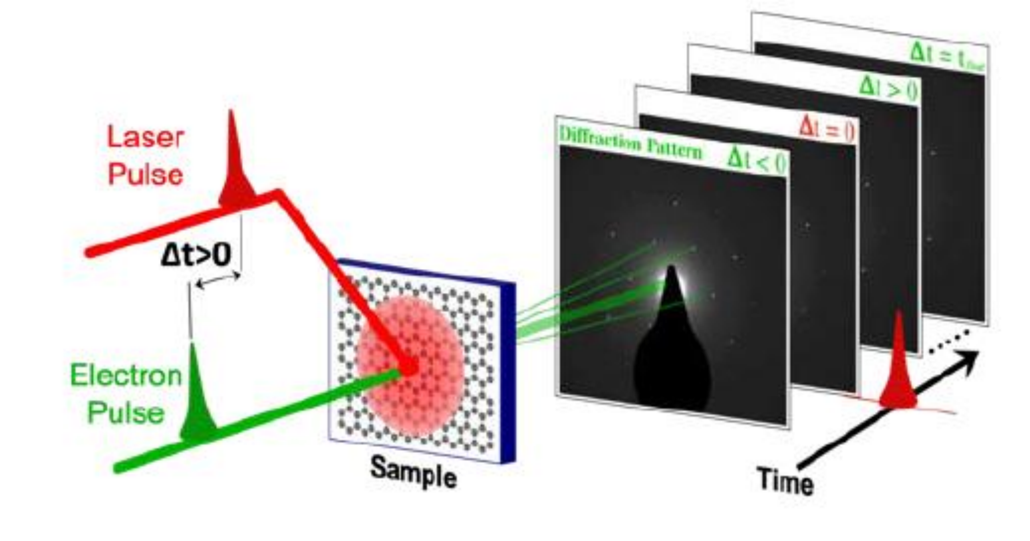
Accelerator on a chip: How it works, SLAC National Accelerator Laboratory. Video from *achip.standford.edu*.

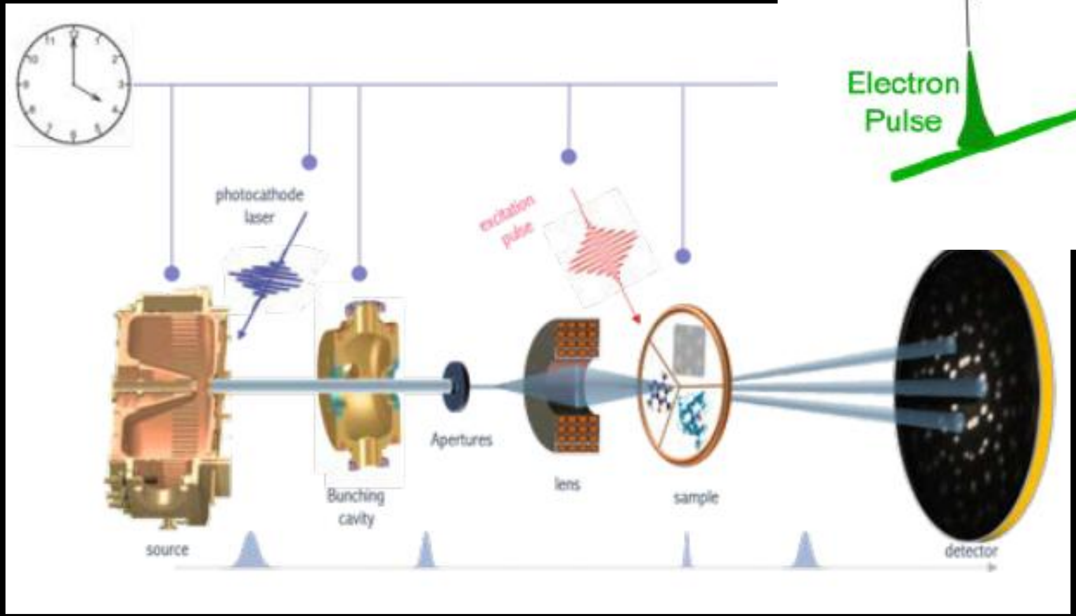
Ultrafast Electron Diffraction (UED)

EuPRAXIA Doctoral Network

Ultrafast Electron Diffraction (UED)

$$\Delta s = \frac{2\pi}{L_{coh}}, L_{coh} = \frac{\hbar}{m_e c}\frac{\sigma_x}{\epsilon_x}$$





$$B_{6D} = \frac{Ne}{\epsilon_{n,x}\epsilon_{n,y}\epsilon_{n,z}} = \frac{I_{rms}}{\epsilon_{n,x}\epsilon_{n,y}\frac{\sigma_E}{mc}}$$

- Temporal resolution 100 fs – 1 ps (jitter < 100 fs)
- Spatial resolution: $\Delta s < 0.01$ Å^{-1}
- Bragg's Law: $|s| = 2|k|\sin\theta$

Filippetto, Daniele, et al. "Ultrafast electron diffraction: Visualizing dynamic states of matter." Reviews of modern physics 94.4 (2022): 045004.

THz Fields for UED

- **Jitter-free**: The terahertz pulse is driven by the pump laser system, generally used for illuminating photocathodes.

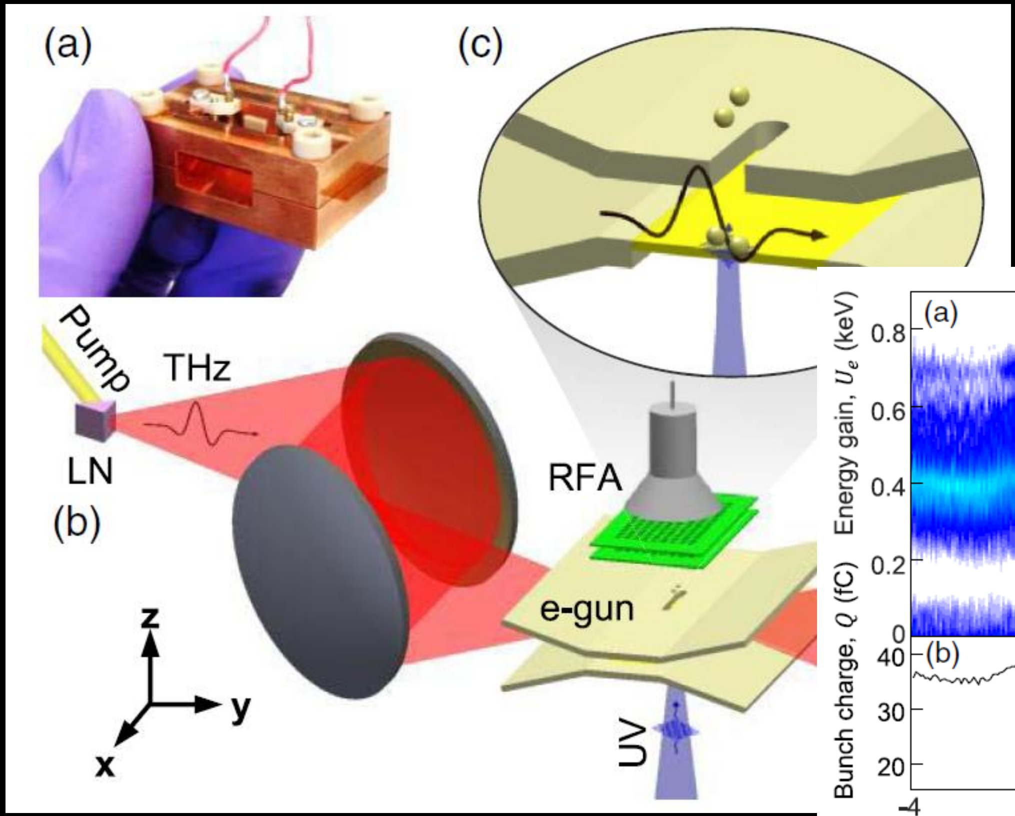
- Higher accelerating gradients, and convenient for manipulation.

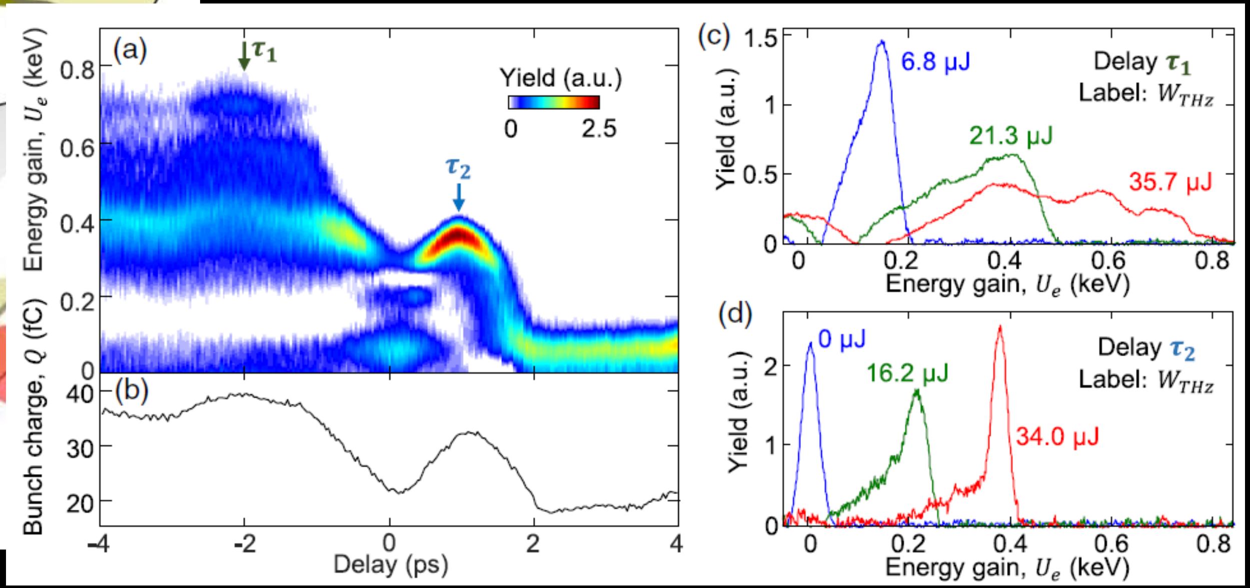
- **Low emittance, ultrashort** electron pulses.

- Compactness.

THz-driven electron gun

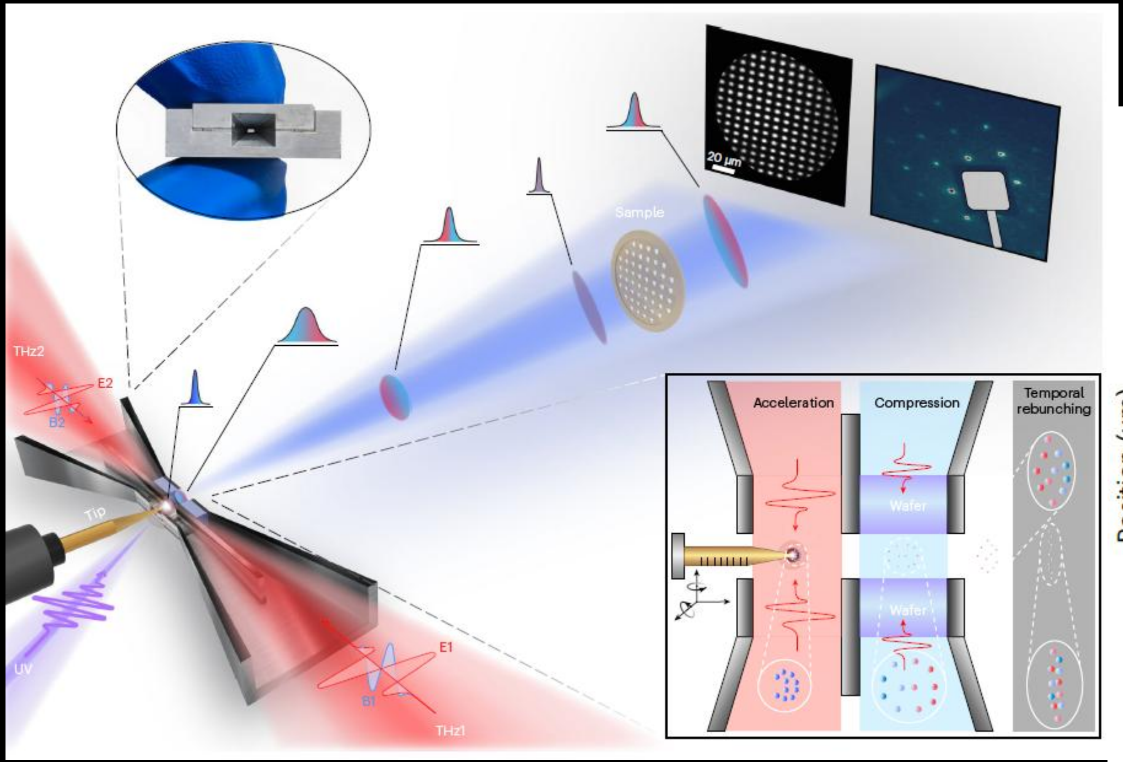
- High Field (> 300 MV/m).
- Few percentage energy spread.
- ~ tens of fC electron bunches.
- LEED.

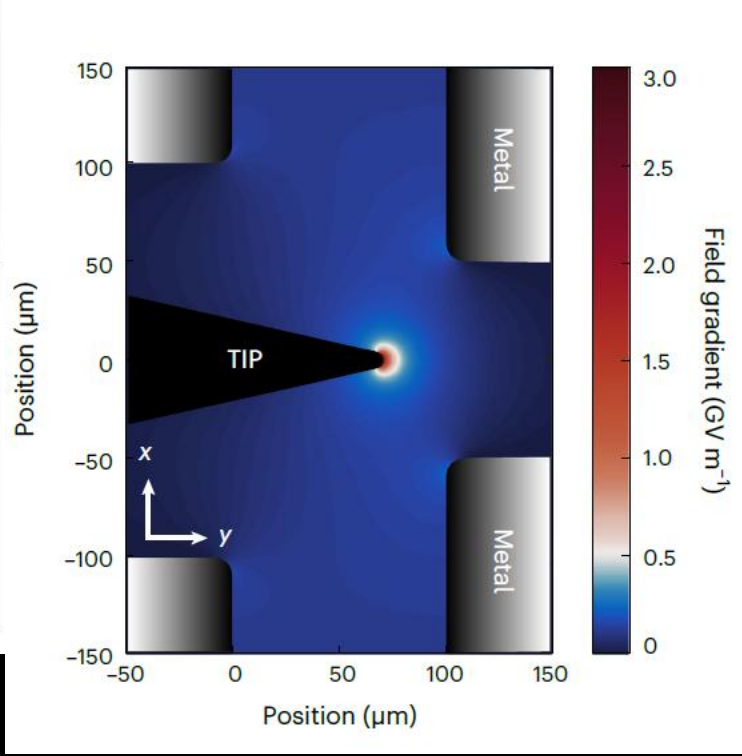




Ronny Huang, W., et al. "Terahertz-driven, all-optical electron gun." Optica 3.11 (2016): 1209-1212.

THz-driven ultrafast photogun





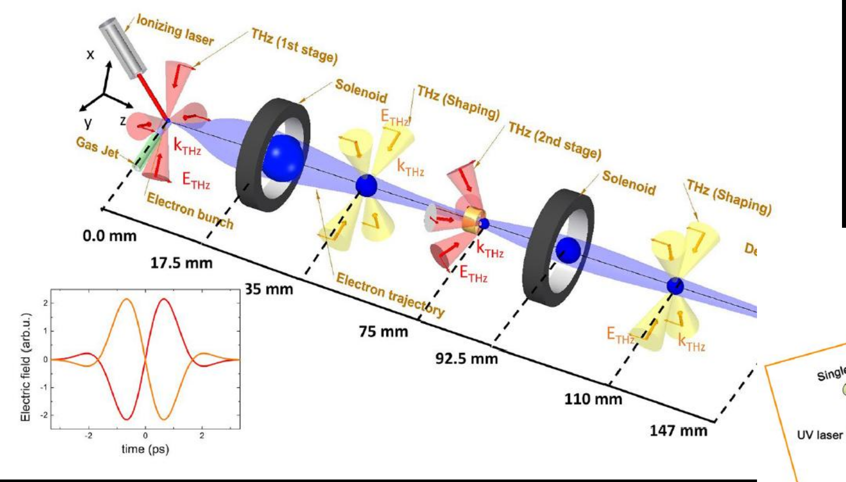
- Ten-fold enhancement thanks to the tip
- Peak acceleration fields ~ 3 GV/m!
- Beam diameter lower thn 90 µm
- Trasv. Emit. < 0.015 mm mrad

Ying, Jianwei, et al. "High gradient terahertz-driven ultrafast photogun." Nature Photonics 18.7 (2024): 758-765.

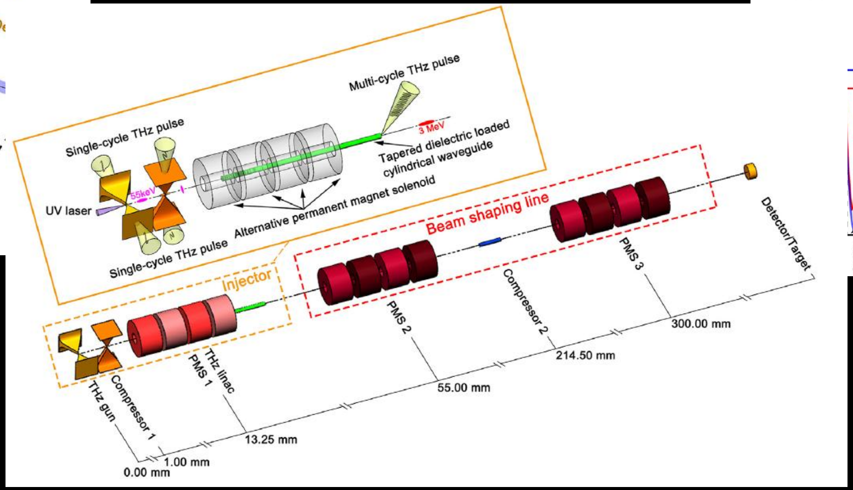
Compact THz-driven electron source

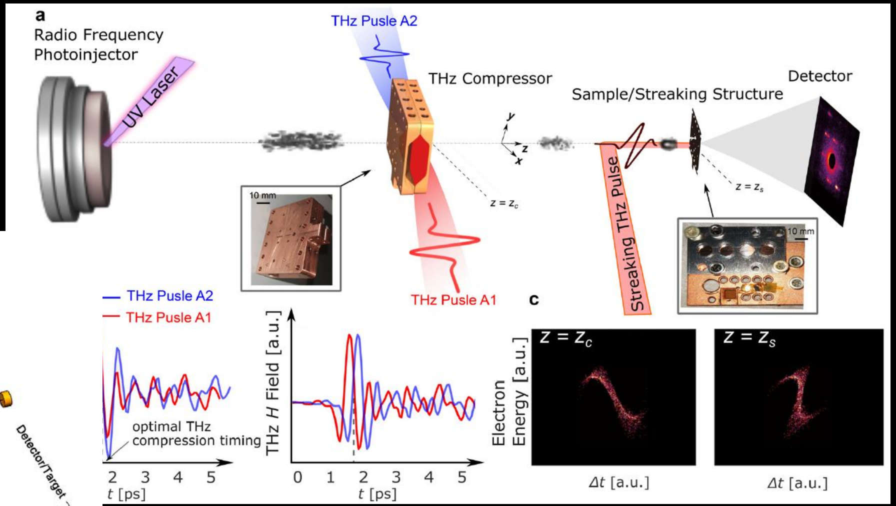
THz-driven relativistic source

Electron bunches for MeV-UED



Compact THz-driven electron source





Turnár, Sz, et al. "Design of a THz-driven compact relativistic electron source." Applied Physics B 127 (2021): 1-7.

Xu, Hanxun, et al. "Towards a compact all-optical terahertz-driven electron source." Frontiers in Physics 11 (2023): 1292194.

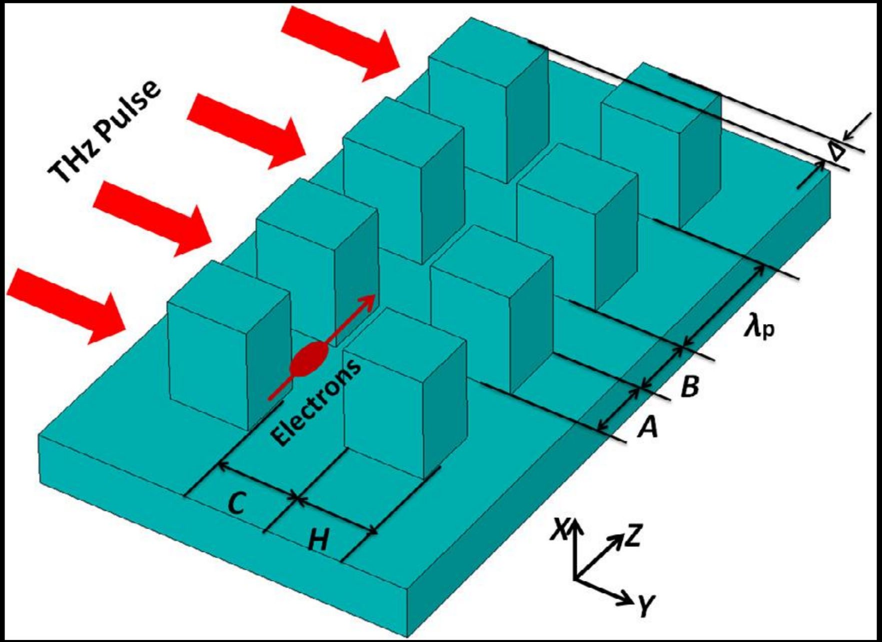
Time-stamping – pixel by pixel representation of temporal dynamics

Othman, Mohamed AK, et al. "Improved temporal resolution in ultrafast electron diffraction measurements through THz compression and time-stamping." Structural Dynamics 11.2 (2024).

Subrelativistic acceleration by DTA

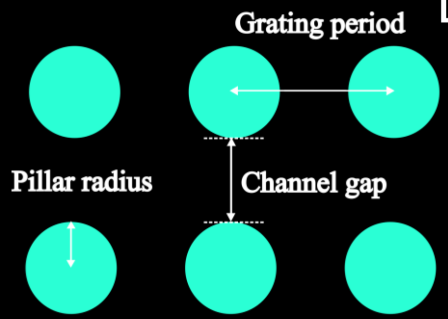
Subrelativistic acceleration by DTA

EuPRAXIA Doctoral Network

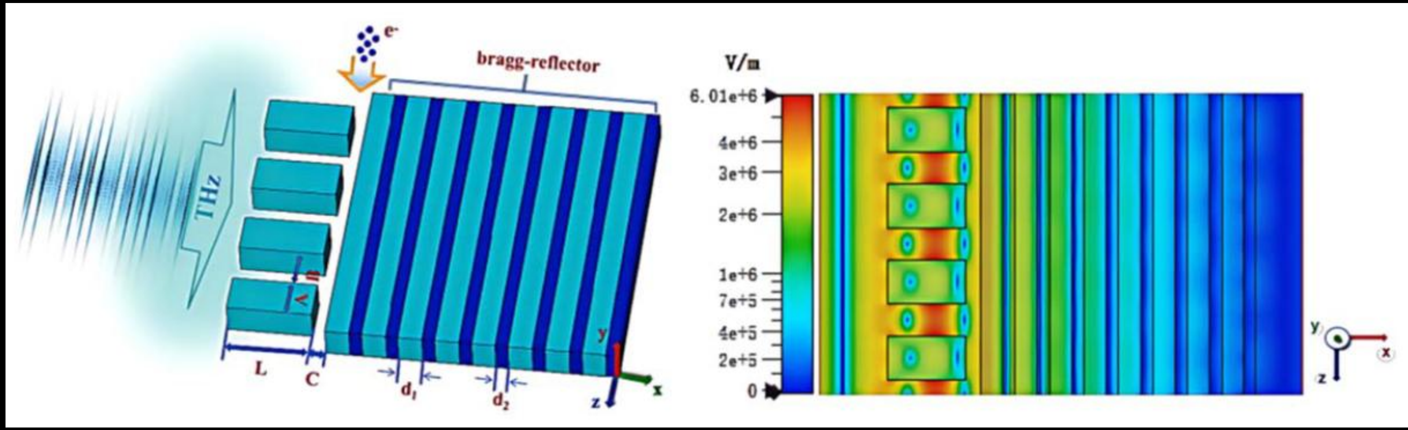


$$G_0 = \frac{q}{\lambda_g}\int_0^{\lambda_g} E_z(z(t),\phi)dz,$$

$$AF = \frac{G_0}{E_{max}}$$



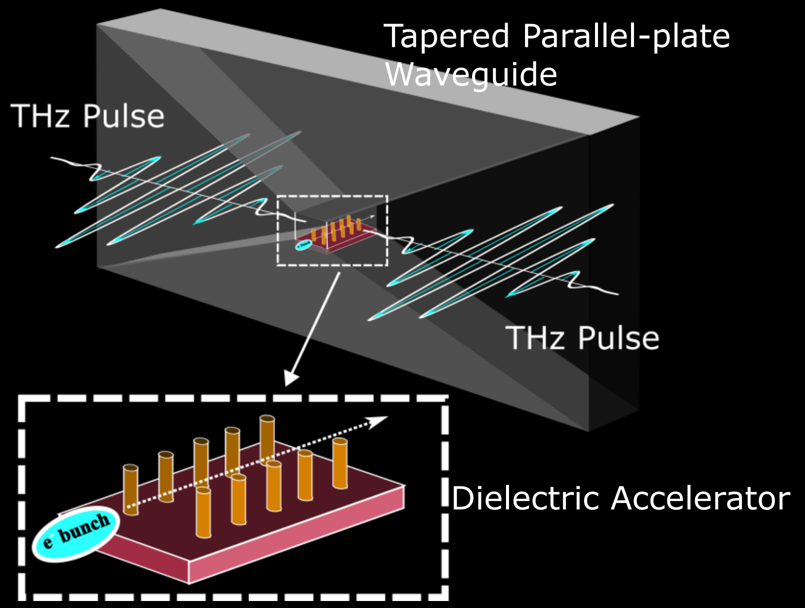
$$\lambda_g = \beta\lambda_{THz}$$



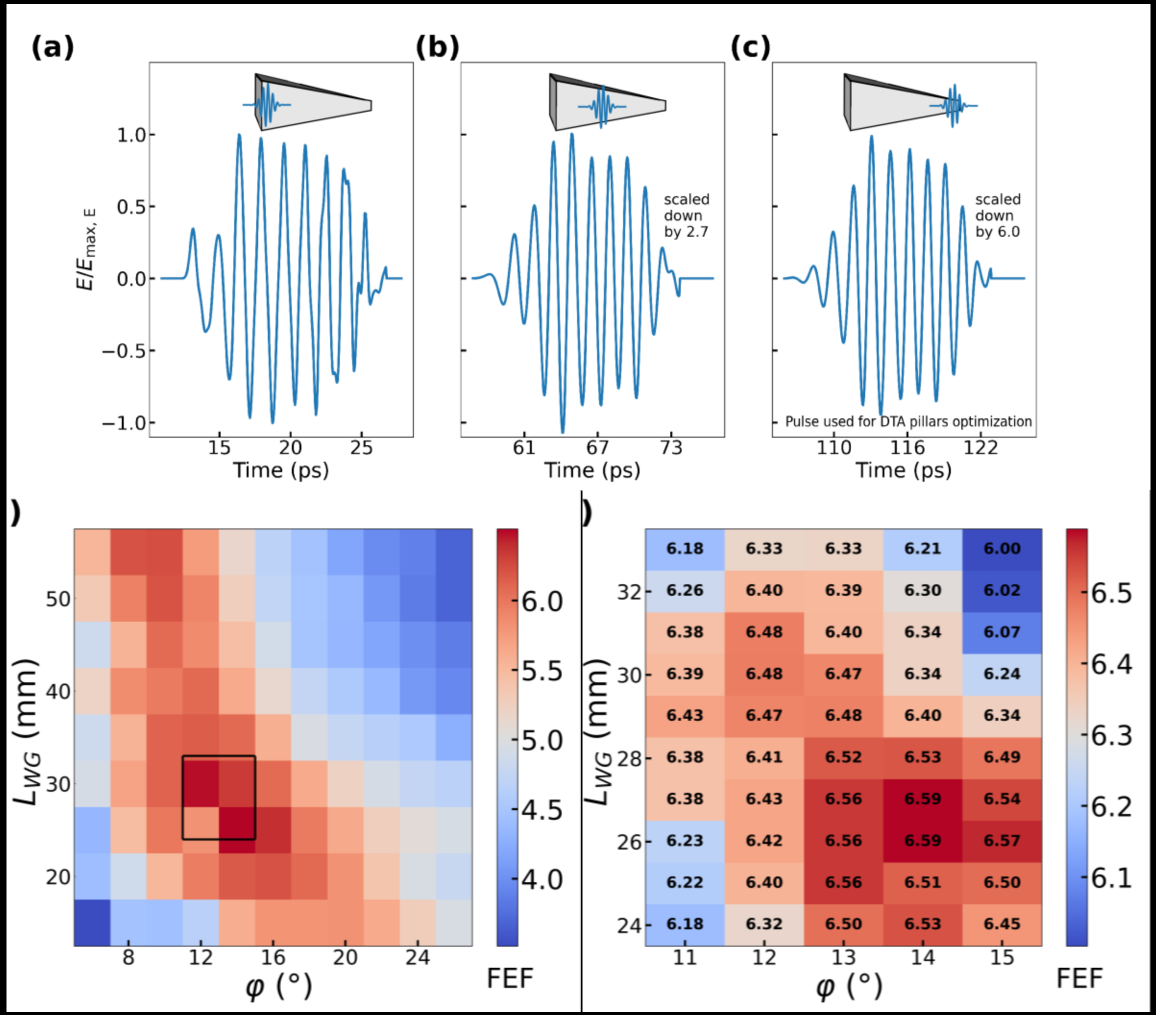
Wei, Y., et al. "Investigations into dual-grating THz-driven accelerators." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 877 (2018): 173-177.

Xiriai, M., et al. "Numerical investigation of a THz-driven dielectric accelerator with a Bragg-reflector for accelerating sub-relativistic electron beams." Physica Scripta 99.7 (2024): 075515.

Parallel-plate Waveguide + DTA



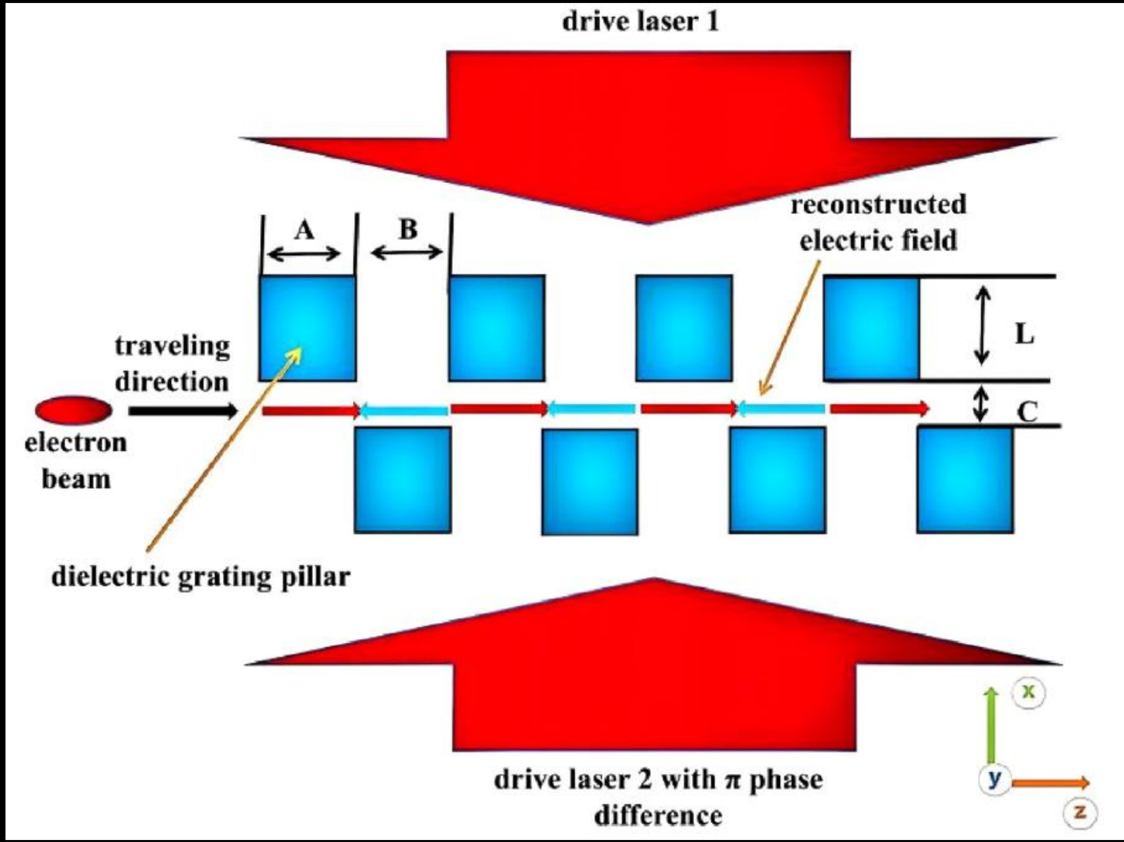
- **Field Enhancement**
- **Efficient Coupling**
- **Phase-mask (for net acceleration)**
- **Transverse and longitudinal focusing (dual-pillar gratings**

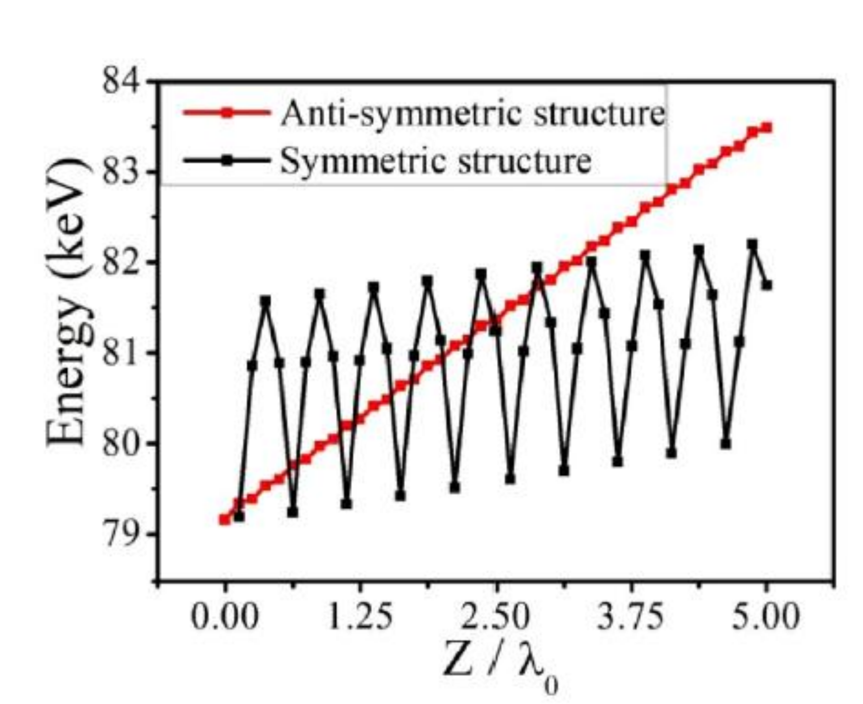


- Top: THz pulse at different positions along the waveguide
- Bottom: Field enhancement factor colormap for the structure parameters waveguide length L_{WG} and angle ϕ

Leiva Genre et. al. 2025, Optics & Laser Technology JOLT-D-25-02556 *(Under Review)*

Subrelativistic accelerator: Improved gradient

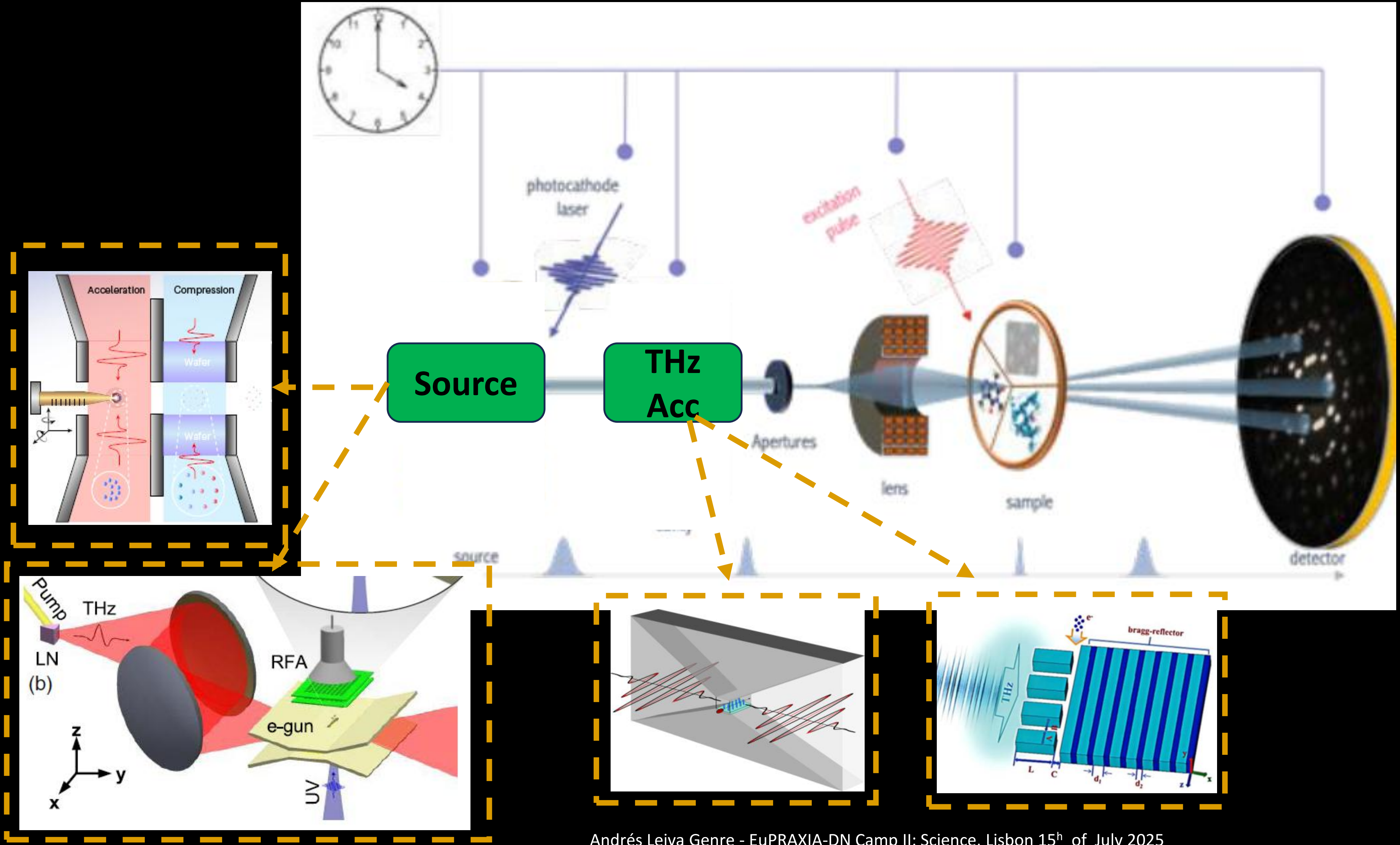




Xiriai, M., et al. "Numerical investigation of an anti-symmetric nanophotonic structure for accelerating sub-relativistic electron beams." Journal of Applied Physics 137.3 (2025).

Proposed setup using DTA

EuPRAXIA Doctoral Network



Solid State: ordering, excitation and emergent phenomena in materials

- Study of macroscopic properties and ordered phase of materials: Interplay of charges, spin, orbital and lattice-structural degrees of freedom

- Condensed matter: Excitation interaction (phonons, charge carriers)

- Structures, dynamics and non-equilibrium properties of materials

Photochemistry and photobiology

EuPRAXIA Doctoral Network

- Molecule light-response: Photosynthesis, vision, DNA photo-damage, light harvesting and storage devices
- Coherent nuclear motion of vibrational wavepackets along both ground and excited states
- Investigation coupled-nuclear electronic motion in excited states
- Capturing relaxation dynamics
- Direct retrieval of three-dimensional structure from diffraction measurements

Conclusions

•THz-driven electron sources enable compact, table-top electron sources with high accelerating gradients (GV/m scale), reducing system size while improving performance.

•These accelerators can potentially provide **sub-100 femtosecond, low-emittance, and high-brightness electron beams.**

•THz-driven beam compression and synchronization techniques also improve temporal precision, enabling direct observation of non-equilibrium states in matter with femtosecond clarity.

•Such enhanced beam parameters open access to previously unresolvable ultrafast processes in:
- •Materials science (ferroelectric switching, phase transitions, coherent phonons),
- •Chemistry (bond breaking/forming, reaction intermediates),
- •Biology (conformational protein dynamics, enzyme activity).

Closing thoughts

“With an extremely fast ‘electron camera’ … researchers have made the first high-definition ‘movie’ of ring-shaped molecules breaking open in response to light. … The fact that we can now directly measure changes in bond distances during chemical reactions allows us to **ask new questions about fundamental processes stimulated by light**.” *https://www6.slac.stanford.edu/news/2019-04-15-slacs-high-speed-electron-camera-films-molecular-movie-hd*

“The electron motion in atoms and molecules is at the heart of all phenomena in nature that occur outside the nucleus” *Hui et. Al., Attosecond electron microscopy*

Closing thoughts

EuPRAXIA Doctoral Network

“With an extremely fast ‘electron camera’ … researchers have made the first high-definition ‘movie’ of ring-shaped molecules breaking open in response to light. … The fact that we can now directly measure changes in bond distances during chemical reactions allows us to **ask new questions about fundamental processes stimulated by light**.” *https://www6.slac.stanford.edu/news/2019-04-15-slacs-high-speed-electron-camera-films-molecular-movie-hd*

“The electron motion in atoms and molecules is at the heart of all phenomena in nature that occur outside the nucleus” *Hui et. Al., Attosecond electron microscopy*

“Accelerator science influenced 28 % of the physics research carried out between the 1938 and 2009, and, in average, it contributed to Nobel prizes in Physics every 2.9 years”
(Haussacker, E.F., Chao, A.W., The influence of accelerator science on Physics research, Phys. Perspect. 13, 146, 2011)

EuPRAXIA

Doctoral Network

This project has received funding from the European Union´s Horizon Europe research and innovation programme under grant agreement no. 101073480.

HUN-REN
Hungarian Research Network

The project has been supported by the TKP2021 funding scheme – (TKP2021 – EGA17).

The project 2024-2.1.1-EKÖP funded by the ministry of culture and innovation, national fund for research, development and innovation, under the University research grant programme EKÖP-24-4 (Szabolcs Turnár).

EuPRAXIA

Doctoral Network

Andrés Leiva Genre, EuPRAXIA-DN, Complex exam 10th of June 2025

SPARE SLIDES

Acquisition Modes in Ultrafast Electron Diffraction: Stroboscopic vs. Single-Shot

EuPRAXIA Doctoral Network

Stroboscopic mode

- Repetition rate: kHz – MHz
- Electron per pulse: << 1 e-
- Temporal resolution: 100 fs
- Sensitivity: 106 – 109 shots, Itot ~ N Isingle
- Spatial resolution: sub-pm
- Trade-offs: long integration times demand sample stability, robust drift control, and mitigation of laser pointing noise

Single-shot mode

- Electron per pulse: 103 – 105 e-
- Temporal resolution: Limited by space-charge broadening Δt ~ (Q/Eacc)1/2
- Signal-to-noise: maximized per shot, no averaging needed
- Trade-offs: Higher emittance and jitter, spatial/coherence degradation, resolution 1-10 ps without compression

Acquisition Modes in Ultrafast Electron Diffraction: Transmission vs Reflection

EuPRAXIA Doctoral Network

Transmission UED

- Sample: thin film (10 – 200 nm up to 1 um) or gas jet
- Probe energy : keV – MeV
- Observables: Bragg spots, diffuse scattering, pair distributions
- Temporal resolution: 100 fs – 1 ps
- Spatial resolution: ~ 1 Angstrom

Reflection UED

- Sample: single crystal or 2D film on substrate
- Probe energy: 30 – 100 keV
- Observables: Surface Bragg peaks, Laue zones
- Surface sensitivity: sub-Angstroms lattice displacements

Optical DLA challenges

The characteristics of IR and optical lasers naturally cause some drawbacks[1]:

LOW BUNCH CHARGES

SUB-MICRON TOLERANCES

SUB-FEMTOSECONDS TIMING REQUIREMENTS

[1] Nanni, Emilio A., et al. "Terahertz-driven linear electron acceleration." Nature communications 6.1 (2015): 8486.

Advantages of THz-driven acceleration and manipulation

- ✓ Shorter wavelengths than RF (reduce the accelerator's size – table-top footprint)

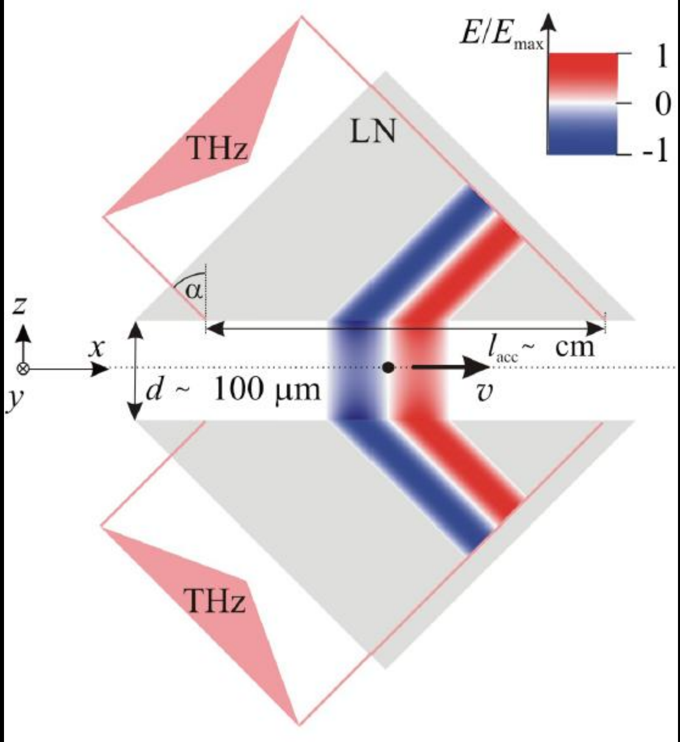
- ✓ Supports whole-bunch acceleration

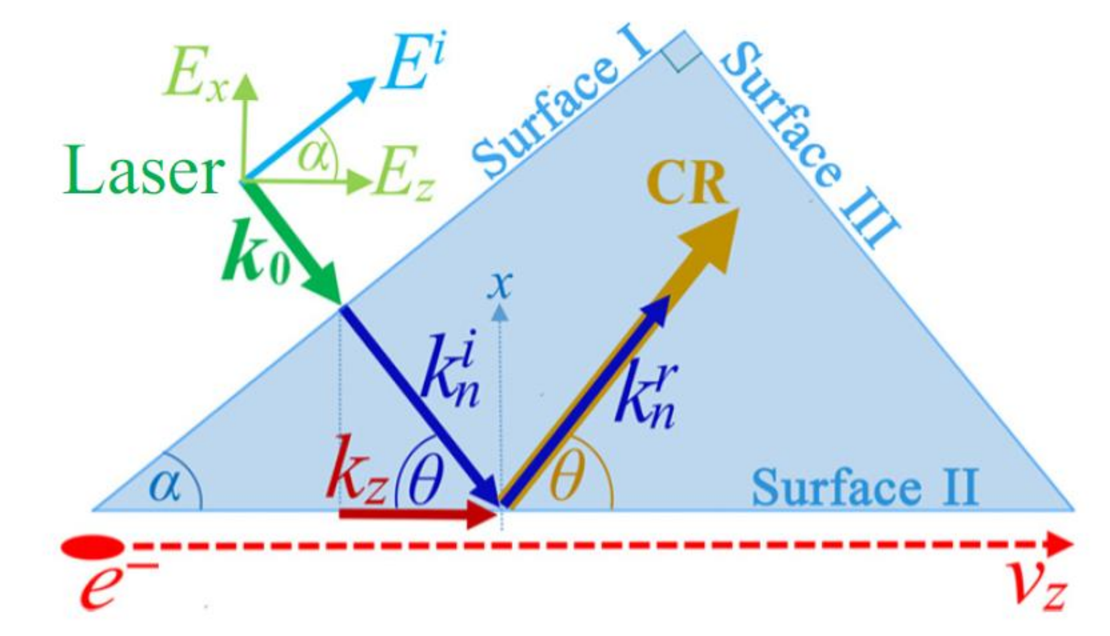
- ✓ Facilitates Structure Manufacturation and Gaps dimensions, allowing greater bunch charges than DLAs

- ✓ THz pulses suited for ultrashort high-charge electron bunches and effective beam manipulation

Inverse-Cherenkov Radiation (ICR) DLA

EuPRAXIA Doctoral Network





Synchronous condition

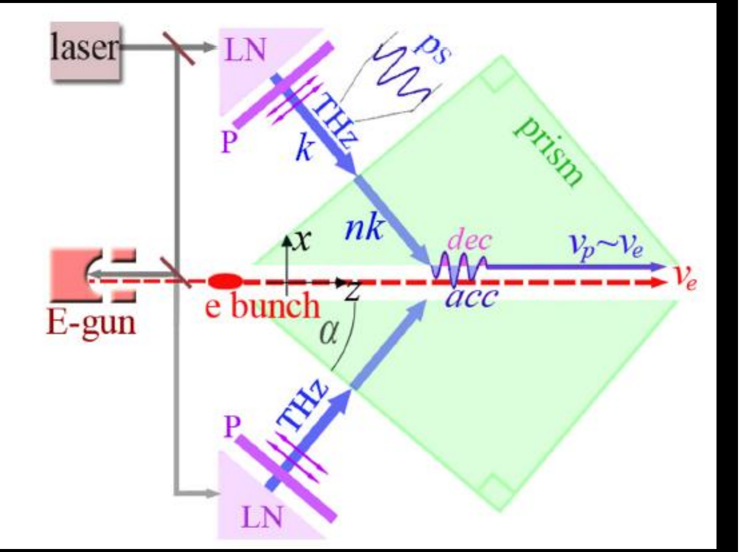
$$v_p = \frac{\omega}{k_z^p} = \frac{\omega}{k_n^i \sin\alpha} = \frac{c}{\sqrt{\varepsilon_r}\sin\alpha} = v_z$$

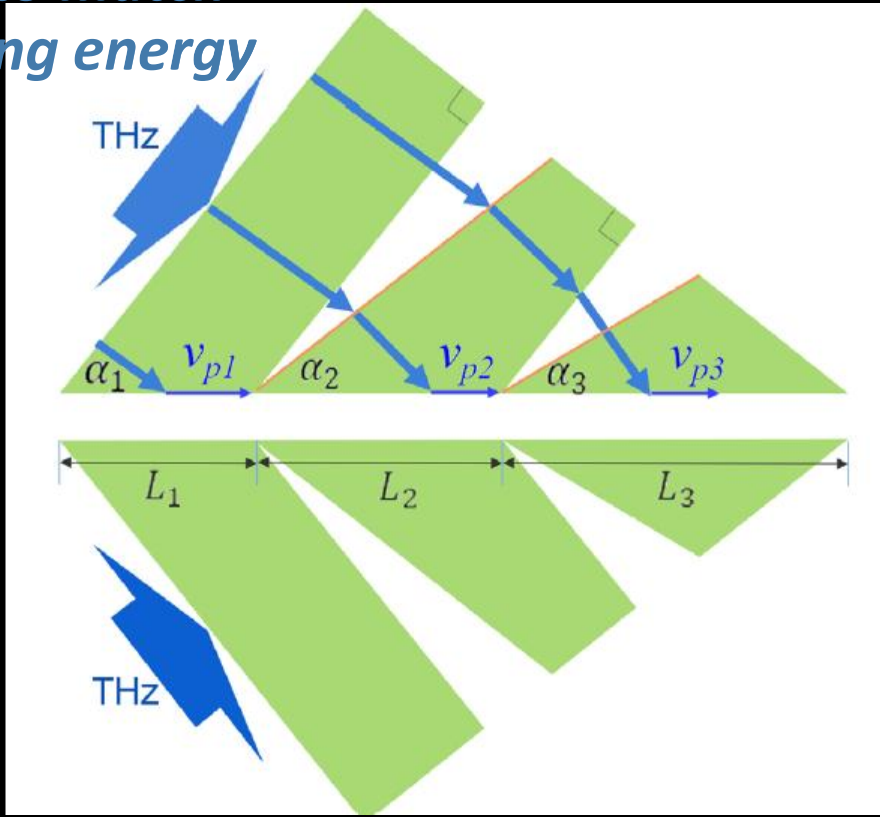
Pálfalvi, L., et al. "Evanescent-wave proton postaccelerator driven by intense THz pulse." Physical Review Special Topics-Accelerators and Beams 17.3 (2014): 031301.

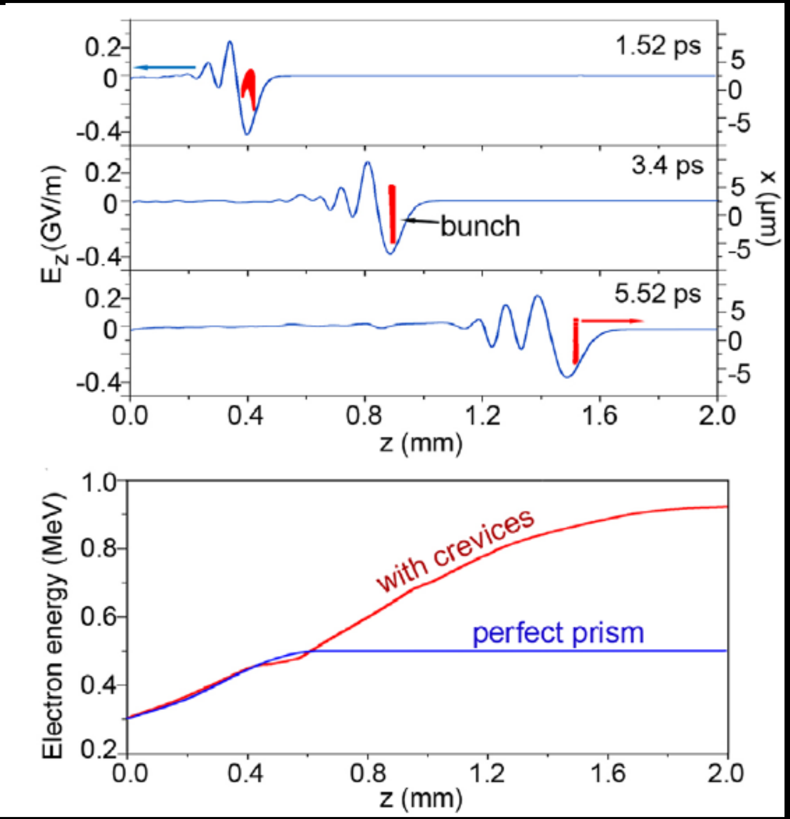
Liu, Weihao, et al. "Microscale laser-driven particle accelerator using the inverse Cherenkov effect." Physical Review Applied 14.1 (2020): 014018.

ICR-DTA Prism Structure

Geometry can be optimized to match electron velocity while gaining energy

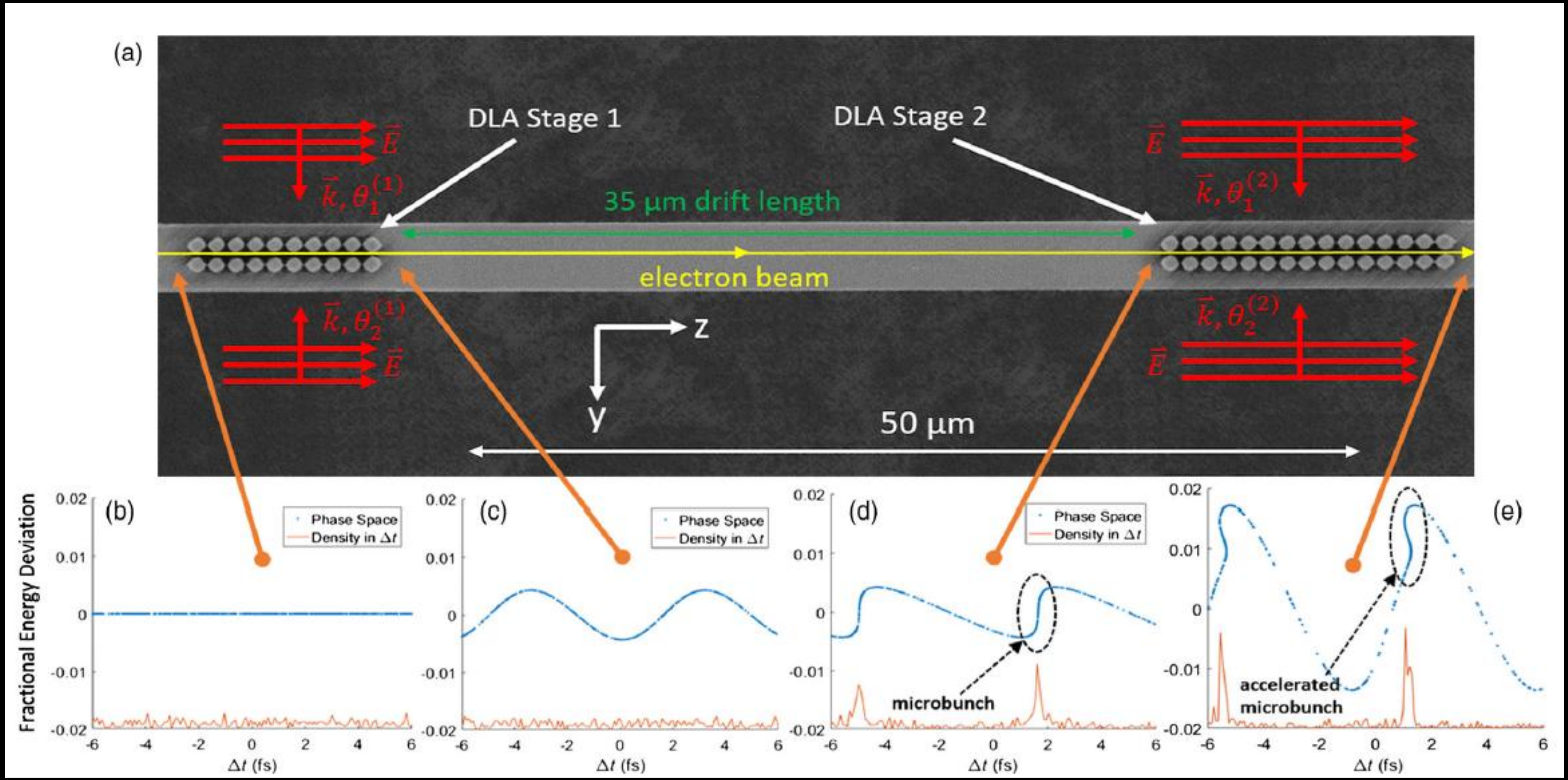






Liu, Weihao, et al. "THz-driven dielectric particle accelerator on chip." Optics Letters 46.17 (2021): 4398-4401.

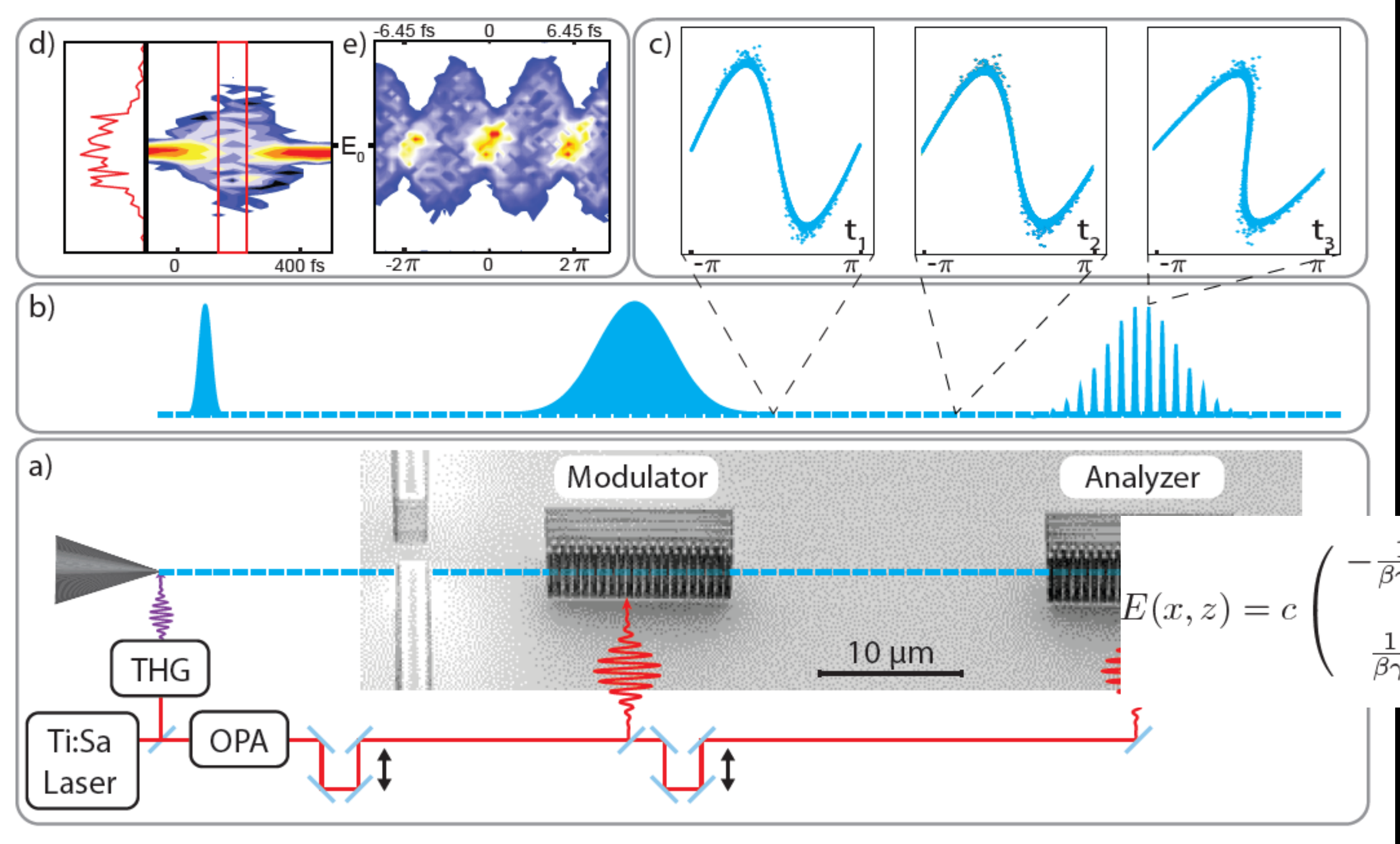
Optical DLAs: Attosecond bunching



Black, Dylan S., et al. "Net acceleration and direct measurement of attosecond electron pulses in a silicon dielectric laser accelerator." Physical review letters 123.26 (2019): 264802.

Optical Attosecond Microbunching

EuPRAXIA
Doctoral Network

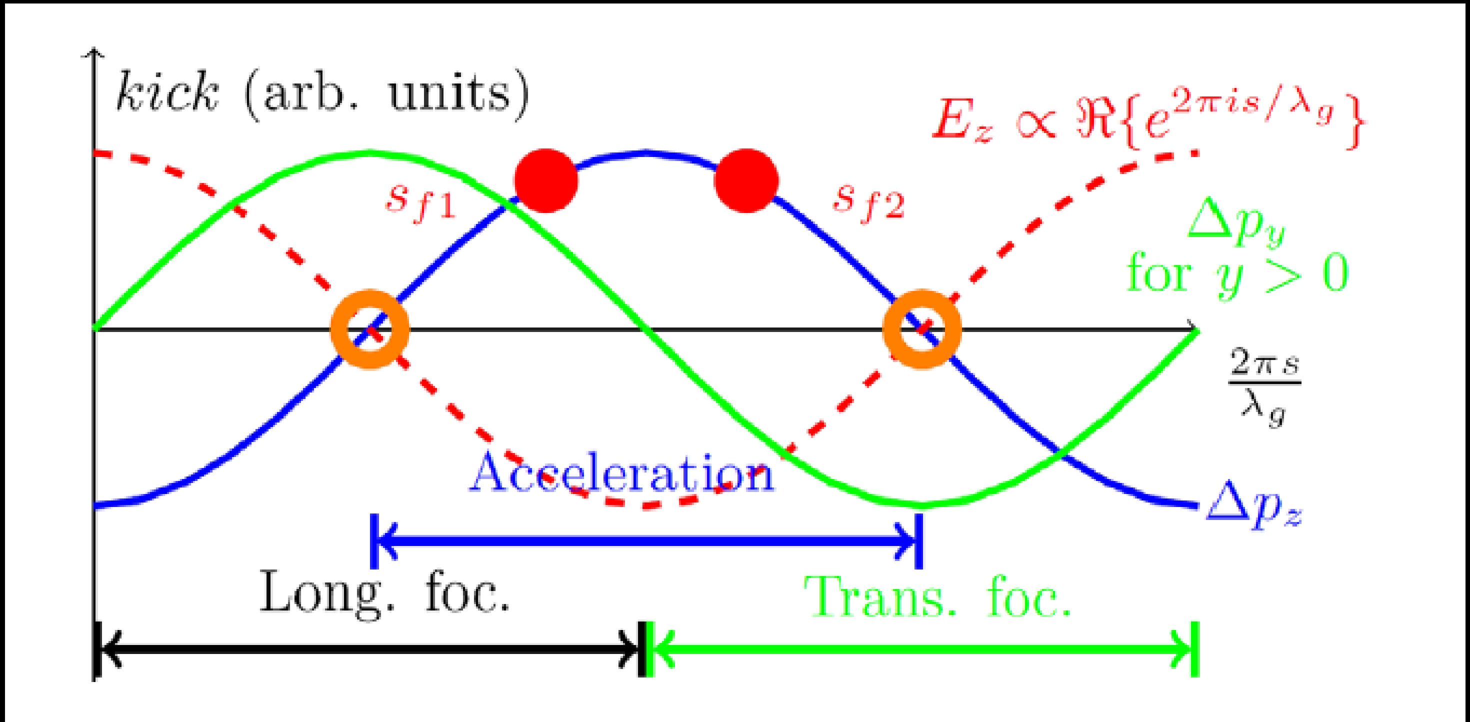


$$E(x,z) = c\begin{pmatrix} -\frac{1}{\beta\gamma^2}\left(C_s \sinh(k_x x) + C_c \cosh(k_x x)\right)\cos(k_z z - \omega t) \\ 0 \\ \frac{1}{\beta\gamma}\left(C_s \cosh(k_x x) + C_c \sinh(k_x x)\right)\sin(k_z z - \omega t) \end{pmatrix}$$

$$\sigma_{FWHM} = (270 \pm 80)\ as$$

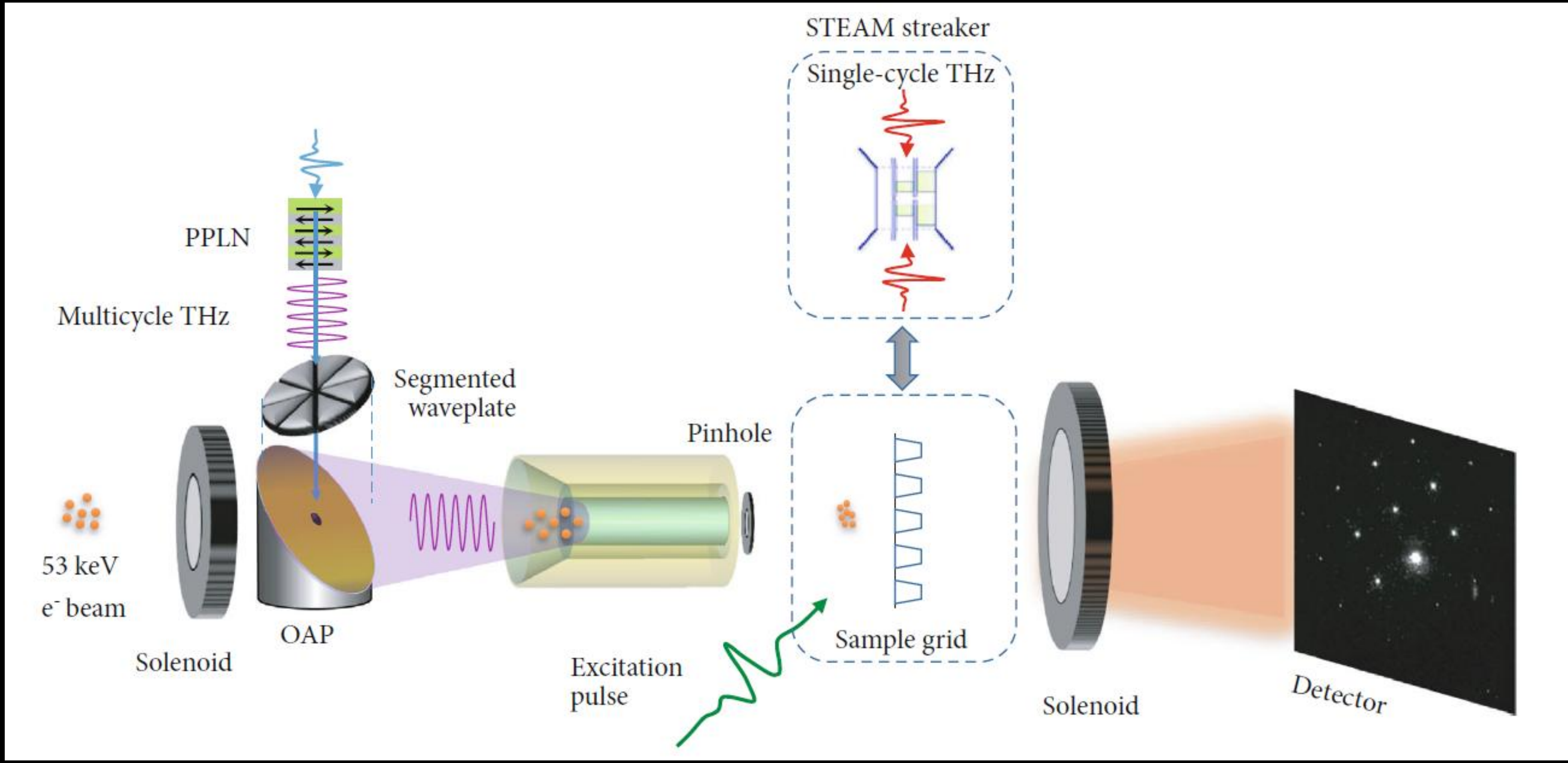
Schönenberger, Norbert, et al. "Generation and characterization of attosecond microbunched electron pulse trains via dielectric laser acceleration." Physical review letters 123.26 (2019): 264803.

Transversal focusing



Overview of electron acceleration and focusing properties as a function of phase. The circles denote the fixed points for different synchronous phase. *Niedermayer, Uwe, et al. "Alternating-phase focusing for dielectric-laser acceleration." Physical review letters 121.21 (2018): 214801.*

THz-driven ultrafast electron source



- 180 fs (FWHM).
- ~ 1 fC.
- 1 kHz repetition rate.
- MeV, sub-30 fs, 10 fC at kHz. repetition rates are predicted.

Zhang, Dongfang, et al. "THz-enhanced DC ultrafast electron diffractometer." Ultrafast Science (2021).

DLA: MOTIVATION

EuPRAXIA Doctoral Network

SIZE

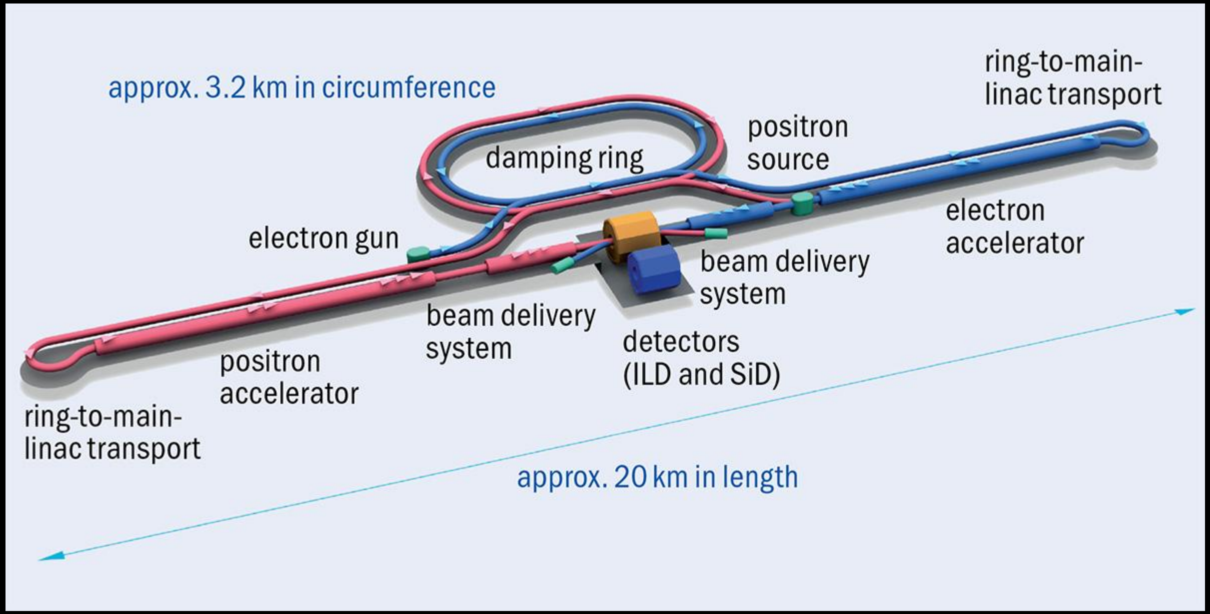
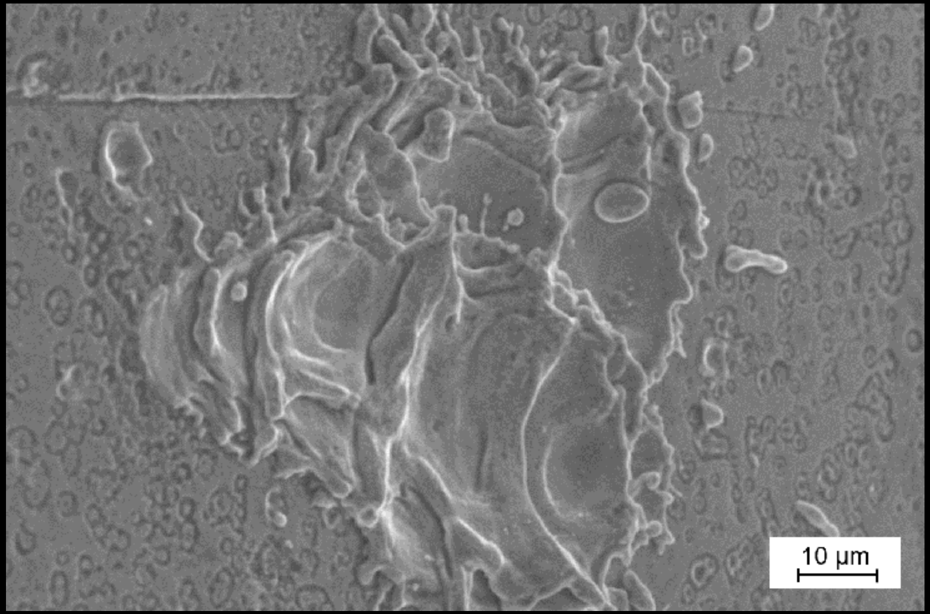


Image taken from CERN Courier. Credit: R Hori / KEK

POWER LIMITATION



Obermair, Christoph, et al. "Explainable machine learning for breakdown prediction in high gradient rf cavities." *Physical Review Accelerators and Beams* 25.10 (2022): 104601.

MOTIVATION

EuPRAXIA Doctoral Network

SIZE

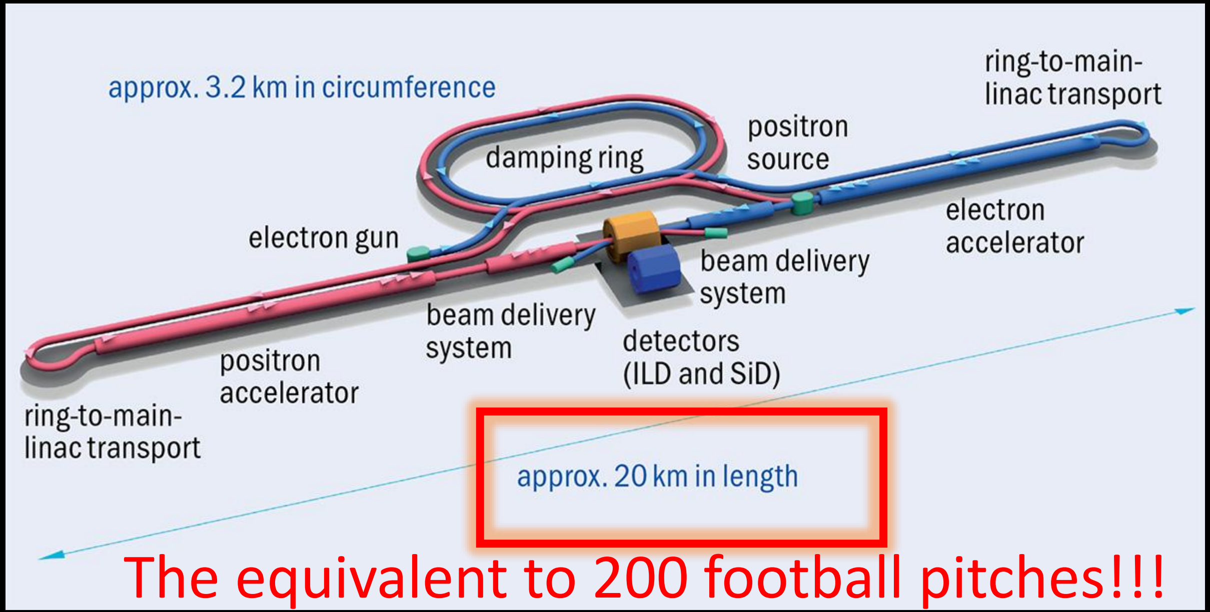
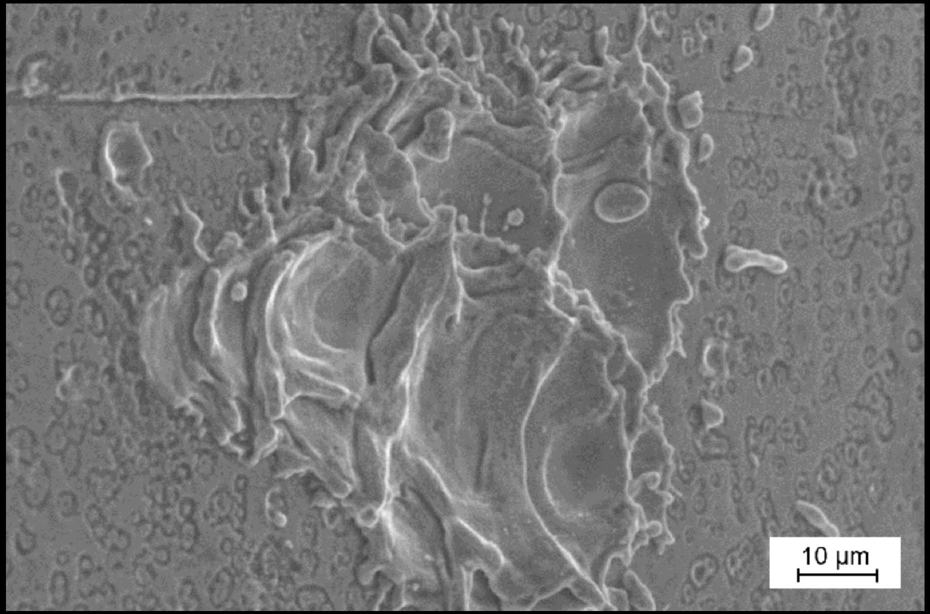


Image taken from CERN Courier. Credit: R Hori / KEK

POWER LIMITATION



Obermair, Christoph, et al. "Explainable machine learning for breakdown prediction in high gradient rf cavities." *Physical Review Accelerators and Beams* 25.10 (2022): 104601.