S2E simulations of THz SASE FEL proof-of-principle experiment at PITZ

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PPS, DESY Zeuthen, 11.09.2018



HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

IR/THz SASE source for pump-probe experiments @E-XFEL

PITZ-like accelerator can enable high power, tunable, synchronized IR/THz radiation



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Planned installation of LCLS-I undulators in PITZ tunnel annex

Will be used for proof-of-principle experiments at PITZ





SASE FEL based on PITZ accelerator and LCLS-I undulators

LCLS-I undulators (available on loan from SLAC) → under study and negotiations

Some Properties of the LCLS-I undulator

Properties	Details		
Туре	planar hybrid (NdFeB)		
K-value	3.49		
Support diameter / length	30 cm / 3.4 m		
Vacuum chamber size	11 mm x 5 mm		
Period length	30 mm		
Periods / a module	113 periods		

Reference: LCLS conceptual design report, SLAC-0593, 2002.





Preliminary conclusions on LCLS-I undulators at PITZ:

- Not such extremely high performance as for the APPLE-II, but is clearly proper for the proof-of-principle experiment!
- 4 nC electron beam transport through the vacuum chamber needs efforts, but seems to be feasible.



 λ_{rad} =100 μ m \rightarrow <Pz>=16.65MeV/c



PITHz: THZ proof-of-principle experiments at PITZ



Beam Dynamics Simulation Setup

ASTRA, SC-optimizer



Photocathode laser



Photocathode laser:

- FT 21.5ps FWHM •
- Ø ≤5mm •
- 4nC ٠

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Gun:

- Ecath=60MV/m (fixed)
- MMMG .

Booster:

- \rightarrow <Pz>=16.7MeV/c + min δ E@undulator? Emax<20MV/m
- Phase=phi2* .



Gun, solenoid, booster parameters





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Emittance at EMSY1 vs. main solenoid

20

Beam at EMSY1 – "ready" for transport

Z=5.277m from the cathode





Based on method of moments w/o space charge

Second order moment of beam distribution function: $M_{\mu\nu} = \langle (\mu - \langle \mu \rangle)(\nu - \langle \nu \rangle) \rangle$, where $\mu, \nu = x, y, p_x, p_y$.

A simple model results in a system of ODE for e.g. x-plane:

 $\frac{dM_{p_{\chi}p_{\chi}}}{d\tau} = 2\kappa \frac{M_{\chi p_{\chi}}}{M_{\chi\chi}}; \frac{dM_{\chi p_{\chi}}}{d\tau} = \frac{M_{p_{\chi}p_{\chi}}}{\gamma}; \frac{dM_{\chi\chi}}{d\tau} = \frac{2}{\gamma} M_{\chi p_{\chi}}$ κ is a space charge related factor (let us assume $\kappa = 0$ for the first approximation), $\tau = ct$. Assuming start from the beam waist ($M_{\chi p_{\chi}}(0) = 0; M_{\chi\chi}(0) = \sigma_0^2$), the solution of the ODE can be represented as:

$$M_{p_x p_x}(\tau) = M_{p_x p_x}(0)$$
$$M_{x p_x}(\tau) = \frac{M_{p_x p_x}(0)}{\gamma}\tau$$
$$M_{x x}(\tau) = \sigma_0^2 + \frac{M_{p_x p_x}(0)}{2\gamma}\tau^2$$

Beam emittance is invariant for these conditions:

$$\varepsilon_{n,x}^2 = M_{xx}M_{p_xp_x}(0) - M_{xp_x}^2 = \sigma_0^2 M_{p_xp_x}^2(0) = const$$



$$M_{\chi\chi}(z) = \sigma_0^2 + \frac{\varepsilon_{n,\chi}^2}{2\gamma\beta^2\sigma_0^2}z^2$$

Denoting $z_A = \frac{\sigma_0^2\beta}{\varepsilon_{n,\chi}}\sqrt{2\gamma}$, one obtains
 $\frac{\sigma}{\sigma_0} = \frac{\sqrt{M_{\chi\chi}(z)}}{\sigma_0} = \sqrt{1 + \frac{z^2}{z_A^2}}$



Based on method of moments w/o space charge

$$M_{\chi\chi}(z) = \sigma_0^2 + \frac{\varepsilon_{n,\chi}^2}{2\gamma\beta^2\sigma_0^2}z^2$$

$$\sigma^2(z=L,\sigma_0) = \sigma_0^2 + \frac{\varepsilon_{n,x}^2}{2\gamma\beta^2\sigma_0^2}L^2$$

 $L = \frac{L_U}{2}$ is a half undulator length,

$$\frac{\partial \sigma}{\partial \sigma_0} = 0 \to \sigma_{0,min} = \sqrt{\frac{\varepsilon_{n,x}L}{\beta\sqrt{2\gamma}}}$$
$$\sigma(z = L, \sigma_{0,min}) = \sqrt{2}\sigma_{0,min} = \sqrt{\sqrt{\frac{2}{\gamma}\frac{\varepsilon_{n,x}L}{\beta}}}$$

Applying obtained beam parameters:

$$\varepsilon_{n,x} = 4 \cdot 10^{-6} m rad$$

 $L = \frac{L_U}{2} = 1.7m$
 $\gamma = 32.6$
 $\beta = 0.9995$
 $\sigma(z = L, \sigma_{0,min}) \approx 1.3mm$

Based on ASTRA simulations with space charge



"Ideal" electron beam:

- Q=4nC
- Temporal: FT, 7ps FWHM
- Transverse phase space: Gaussian
- <Pz>=16.7MeV/c
- ε(z=0)=4 mm mrad



$$GF(X_{rms,0}) = \sqrt{\frac{1}{L} \int_0^L X_{rms}^2 dz}$$



Based on ASTRA simulations with space charge



100 50 p_× (mrad) -50 -100L -2 -1 2 0 1 - 3 x (mm) 1.2 5 0.8 **size (mm)** 0.6 E 3.8 4 Xrms(1) 3.6 H 04 Xrms(0) --- Xemit(1) 3.4 0.2 ---Xemit(0) 3.2 0 0.5 1.5 2 2.5 3.5 0 z (m) 100 4 50



100 5 50 p_× (mrad) -100 2 -2 -1 0 1 3 x (mm)

"Ideal" (Gaussian-FT) electron beam:

- Q=4nC ٠
- <Pz>=16.7MeV/c ٠
- ε~4 mm mrad ٠ can be transported through pipe:
- L=3.4m ٠
- Ø5mm ٠

S2E simulations of THz SASE FEL at PITZ | M. Krasilnikov | PPS, 11.9.2018





PITZ Beam from the cathode → tunnel wall

ASTRA→ SC-optimizer



NB: ASTRA Space Charge 3D: 200k particles $\rightarrow N_{x,y,z}=16 \rightarrow 13$ part/cell 200k particles $\rightarrow N_{x,y,z}=32 \rightarrow 191$ part/cell





Quadrupole "recalibration"

- SC-optimizer → Hard edge model
- A. Matvienko "Effective length of the thick lens": $L_{eff} = \frac{6 \int_{-\infty}^{\infty} \left[\int_{-\infty}^{z} g(z_1) dz_1 \cdot \int_{z}^{\infty} g(z_2) dz_2 \right] dz}{\left[\int_{-\infty}^{\infty} g(z) dz \right]^2}$
- ASTRA → Measured gradient Q3.dat









PITZ Beam from the cathode → tunnel wall

ASTRA check





PITZ Beam from the cathode → tunnel wall

Beam emittance using SC-optimizer and ASTRA



S2E simulations: 4nC 16.7MeV/c beam transport from the cathode till and through the tunnel wall \rightarrow OK



By(z) field profile measurements done on 02.10.2013 at SLAC for the undulator L143-112000-07 after the final tuning



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By(z) field profile measurements done on 02.10.2013 at SLAC for the undulator L143-112000-07 after the final tuning

Based on file x+00000_y+000_bscanz.dat (communication with Heinz-Dieter Nuhn from 06.07.2018)



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-0.002

-0.004

-0.006

-0.008

4.4

Fourier Analysis



Fourier Analysis



Field integrals of the undulator:



"Improving " the field profile

The procedure to generate infinitely smooth $B_v(0,0,z)$ distribution antisymmetric w.r.t. z=0 includes several steps:

- Rough centering of the distribution $B_{y,raw}(z)$, so $B_{y,raw}(-z) \approx -B_{y,raw}(z)$,
- Determination of $N_U = L/\lambda_U$ the for Fourier transformation of the measured data,
- Determination of the background based on the left $B_{y,bkg-left} = B_{y,bkg}(-L/2)$ and right

 $B_{y,bkg-right} = B_{y,bkg}(L/2)$ using linear dependence: $B_{y,bkg}(z) = B_{y,bkg-left} + \frac{B_{y,bkg-right} - B_{y,bkg-left}}{L}$.

- Subtraction of the background: $B_{y,1}(z) = B_{y,raw}(z) B_{y,bkg}(z)$
- Fine centering of the obtained distribution $B_{y,1}(z_1 = z z_0)$, so $B_{y,1}(z_1 = 0) = 0$,
- Symmetrizing the distribution $B_{y,2}(z_2) = \frac{B_{y,2}(z_2) B_{y,2}(-z_2)}{2}$ on the mesh z_2 which includes $z_2 = 0$ explicitly.

All these steps were included in the optimization procedure with following optimization parameters:

$$\{N_U, B_{y,bkg-left}, B_{y,bkg-right}\}, \text{ minimizing } : \Phi(N_U, B_{y,bkg-left}, B_{y,bkg-right}) = \sum_{n=1}^{N_h \cdot N_U} \frac{(-1)^n}{\pi n} \tilde{b}_n,$$

where $\tilde{b}_n = \frac{2}{N_U \lambda_U} \int_{-\frac{N_U \lambda_U}{2}}^{\frac{N_U \lambda_U}{2}} B_{y,2}(x=0, y=0, z_1) \sin\left(\frac{2\pi n z_1}{N_U \lambda_U}\right) dz$,

and the number of harmonics N_h is taken to be high enough ($N_h > 10$, typically, $N_h = 17$).





$$B_{y,2}(0,0,z) = \sum_{n=1}^{N_h \cdot N_U} \left\{ \tilde{a}_n \cos\left(\frac{2\pi nz}{N_U \lambda_U}\right) + \tilde{b}_n \sin\left(\frac{2\pi nz}{N_U \lambda_U}\right) \right\}$$

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3D field map generation

Scalar magnetic potential $\Psi(y, z)$ for the case of the field which is symmetric in the horizontal plane and homogeneous in horizontal:

$$\Psi(y,z) = \sum_{m=0}^{\infty} (-1)^m \frac{d^{2m} B_{y,2}(0,0,z)}{dz^{2m}} \cdot \frac{y^{2m+1}}{(2m+1)!}.$$
Applying differentiation to
$$M_{N_U\lambda_U} = \sum_{n=1}^{N_h \cdot N_U} \left\{ \tilde{a}_n \cos\left(\frac{2\pi nz}{N_U\lambda_U}\right) + \tilde{b}_n \sin\left(\frac{2\pi nz}{N_U\lambda_U}\right) \right\}.$$

$$\frac{d^{2m} B_{y,2}(0,0,z)}{dz^{2m}} = \sum_{n=1}^{N_h \cdot N_U} (-1)^m \left(\frac{2\pi n}{N_U\lambda_U}\right)^{2m} \left\{ \tilde{a}_n \cos\left(\frac{2\pi nz}{N_U\lambda_U}\right) + \tilde{b}_n \sin\left(\frac{2\pi nz}{N_U\lambda_U}\right) \right\}.$$

$$\Psi(y,z) = \sum_{n=1}^{N_h \cdot N_U} \sum_{m=0}^{\infty} \left(\frac{2\pi n}{N_U\lambda_U}\right)^{2m} \left\{ \tilde{a}_n \cos\left(\frac{2\pi nz}{N_U\lambda_U}\right) + \tilde{b}_n \sin\left(\frac{2\pi nz}{N_U\lambda_U}\right) \right\} \cdot \frac{y^{2m+1}}{(2m+1)!}.$$
Components of the magnetic field $\vec{B} = \nabla \Psi$ can be calculated:

$$\begin{split} B_{x} &= \frac{\partial \Psi(y,z)}{\partial x} = 0, \\ B_{y} &= \frac{\partial \Psi(y,z)}{\partial y} = \sum_{n=1}^{N_{h} \cdot N_{U}} \left[\left\{ \tilde{a}_{n} \cos\left(\frac{2\pi nz}{N_{U}\lambda_{U}}\right) + \tilde{b}_{n} \sin\left(\frac{2\pi nz}{N_{U}\lambda_{U}}\right) \right\} \cdot \sum_{m=0}^{\infty} \left(\frac{2\pi n}{N_{U}\lambda_{U}}\right)^{2m} \frac{y^{2m}}{(2m)!} \right], \\ B_{z} &= \frac{\partial \Psi(y,z)}{\partial z} = \sum_{n=1}^{N_{h} \cdot N_{U}} \left[\left\{ -\tilde{a}_{n} \sin\left(\frac{2\pi nz}{N_{U}\lambda_{U}}\right) + \tilde{b}_{n} \cos\left(\frac{2\pi nz}{N_{U}\lambda_{U}}\right) \right\} \cdot \sum_{m=0}^{\infty} \left(\frac{2\pi n}{N_{U}\lambda_{U}}\right)^{2m+1} \frac{y^{2m+1}}{(2m+1)!} \right]. \end{split}$$



3D field map generation

Utilizing

$$\sum_{m=0}^{\infty} \frac{\xi^{2m}}{(2m)!} = \cosh \xi, \quad \sum_{m=0}^{\infty} \frac{\xi^{2m+1}}{(2m+1)!} = \sinh \xi,$$

Vertical and longitudinal components can be finally re-written:

$$B_{y} = \sum_{n=1}^{N_{h} \cdot N_{U}} [\{\tilde{a}_{n} \cos(k_{n}z) + \tilde{b}_{n} \sin(k_{n}z)\} \cdot \cosh(k_{n}y)],$$

$$B_{z} = \sum_{n=1}^{N_{h} \cdot N_{U}} [\{-\tilde{a}_{n} \sin(k_{n}z) + \tilde{b}_{n} \cos(k_{n}z)\} \cdot \sinh(k_{n}y)],$$

where $k_n = \frac{2\pi n}{N_U \lambda_U}$ is the wavenumber of the *n*-th Fourier harmonic.







On-axis particle trajectory in the undulator

ASTRA reference particle and CST tracking



Vertical on-axis trajectory \rightarrow y=0



Off-axis particle trajectory in the undulator

ASTRA reference particle



case	X(0), mm	X'(0), mrad	Y(0), mm	Y'(0), mrad
0	0	0	0	0
1	1	0	0	0
2	1	-0.5	0	0
3	0	0	1	0
4	0	0	1	-0.5
5	0.7	-0.35	0.7	-0.35



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Off-axis particle trajectory in the undulator

ASTRA reference particle



case	X(0), mm	X'(0), mrad	Y(0), mm	Y'(0), mrad
0	0	0	0	0
1	1	0	0	0
2	1	-0.5	0	0
3	0	0	1	0
4	0	0	1	-0.5
5	0.7	-0.35	0.7	-0.35







Off-axis particle trajectory in the undulator

ASTRA reference particle





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Beam matching into the undulator

ASTRA simulations with space charge and 3D undulator field map



New transport / matching

Further "through the wall" + prepare for asymmetric matching into the undulator





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Electron beam transport for LCLS-I undulator option at PITZ

2 solution s (M1 and M2) for the matching into the undulator \rightarrow beam size



Electron beam transport for LCLS-I undulator option at PITZ

2 solution s (M1 and M2) for the matching into the undulator \rightarrow emittance



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CST Particle Studio Simulations

More correct space charge estimations + vacuum chamber impact

• Still on-going...

Beam at undulator entrance

ASTRA monitors at z=27.15m





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GENESIS1.3 Simulations

ASTRA at 27.15m → GENESIS1.3

See slides from Prach

DÈŚ

Beam at undulator exit

ASTRA monitors at z=30.7m



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Conclusions

Star-to-End simulations for the proof-of-principle experiment for SASE THz FEL at PITZ using LCLS-I undulator

- PITZ Setup:
 - Gun: 60MV/m, 0deg
 - Photocathode laser: Ø5mm, 21.5ps FWHM, 4nC
 - CDS booster setup: 12.6MV/m, -24deg → 16.7MeV/c + min dE@~undulator
 - Main solenoid: MaxB(1)=-0.21285T (~365A) $\rightarrow \epsilon_{xy}$ (EMSY1)~4.6 mm mrad
 - Transport: 3 quad. triplets \rightarrow transport through the tunnel wall (1.5m)
 - Transport: +1 quad triplet to match into undulator
- Undulator field:
 - Based on measured profile $B_{y}(z,0,0)$
 - Treated (improved) profile to minimize field integrals
 - 3D field map reconstructed → CST and ASTRA
- Tracking beam through the undulator:
 - On-axis reference particle: CST Trk $\leftarrow \rightarrow$ ASTRA with 3D field map
 - Off-axis reference particle in ASTRA to find initial guess for matching
 - 4nC beam by ASTRA (with space charge*) → M1 and M2 found



PITHz: THZ proof-of-principle experiments at PITZ (LCLS-I-und)

Current status (10.09.2018) and outlook

Open questions

- Refine (improve) preliminary optimum solution:
 - Matching after the wall and between U1 and U2 (cross-check with PIC solver)
 - Modeling and optimization of the collimator section
 - ...
- Realistic PC laser parameters Ø3-4mm, other temporal profiles, core+halo (using experimental data)
- Scale / re-optimize setup for λ_{rad} =50-60 μ m
- Prepare experimental program to check 4nC electron beam transport
- Modeling of the THz measurement setup (together with FLASH, N.Stojanovic?)
- Waveguide effects in the THz SASE FEL (together with G.Geloni?)
- Undulator radiation from short bunches
- Seeding option simulations (modulated PC laser based on input from IAP)
- BC design (pool of available magnets?)
- 2nd CDS booster?
- ...

Expected results

- PITZ layout update: new quads, steerers, collimator(s) and diagnostics → prepared for technical design
- Realistic modeling of high charge beam dynamics in the PITZ beamline
- Prepared setups for λ_{rad} =50-100 μ m for experimental tests

• ...



Mini-workshop on proof-of-principle SASE THz FEL at PITZ

 $1\!\!\!/_2$ - 1 day in the 1st $1\!\!\!/_2$ of October

- PITZ accelerator (general layout and parameters)
- Preliminary simulations for THz options at PITZ, experimental results on THz CTR/CDR
- Proposals for proof-of-principle experiments using LCLS-I undulator(s)
- Start-to-end simulations for the proof-of-principle experiments (SASE THz FEL)
- Possible critical problems (real beam transport, wakefield, waveguide regime, etc.)
- Experimental program on the electron beam characterization (4nC emittance and transport)
- PITZ layout modification for LCLS-I undulator installations
- Required electron beam diagnostics
- Machine protection system (BLM, collimator, etc.)
- Required THz diagnostics
- Other options with LCLS-I undulator (undulator radiation with short bunches, seeding, etc.) and required components (e.g., bunch compressor)
- Technical issues (construction, electronics, controls)
- Possible timeline



0.1 mm rms waist \rightarrow not optimum





Electron beam transport for LCLS-I undulator option at PITZ

2 solution s (M1 and M2) for the matching into the undulator \rightarrow beta functions



