

Towards building and operating the brightest x-ray synchrotron radiation source of the future

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Contents

- PETRA IV project overview
- Historical background and lattice design principles for ultra-low emittance electron rings
- Candidate lattices for the PETRA upgrade
- Additional factors Influencing beam parameters
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- Software, HL controls and machine learning
- Conclusion/outlook



- HEP (Positron-Electron Tandem Ring Accelerator) 1978-1986, 1990-2007 (as HERA injector)
- SR source TDR 2004 (DESY 2004-035), Commissioned 2009 (K. Balewski, proc. IPAC'10)
- Staged extension project from 2014 (W. Drube et al., 2016 <u>https://doi.org/10.1063/1.4952814</u>)







TABLE 1 PETRA III parameters incl. extension

Parameter			
Energy	(5	GeV
Circumference	23	04	m
Emittance (hor. / vert.)	1.2/	0.012	nm rad
Total current	10	00	mA
Number of bunches	960	40	
Bunch population	0.5	12	$10^{10} e^{-1}$
Bunch separation	8	192	ns



- The extension project still ongoing, IDs/beamlines being added and commissioned
- Emittance reduction potential of the present lattice with a different phase advance ~500 pm
- With the new generation of machines (MAX-IV, ESRF-EBS, APS-U, Spring8-II, Sirius, Elettra and others) a much more significant emittance reduction will be required by highend users (e.g. coherence applications)
- ESRF-EBS is already starting installation
- To seamlessly continue the SR research programme, DESY will need to put a new machine in operation by late 2020s







Parameters and parameter range, status February 2018:

https://confluence.desy.de/display/PetralV/Accelerator+design

PETRA IV Parameter		
Energy	6 GeV	
Current	200 mA	
Number of bunches	~ 2000	
Emittance horz.	~20 pm rad	(10 – 30 pm rad)
vert.	~20 pm rad	(10 – 30 pm rad)
Bunch length	< ~100 ps FWHM	



Present goals for PETRA IV: 2019 CDR 2021 TDR 2024 Start construction 2026 Start operation



Brillance: > 10²² Photons / (sec mrad² mm² 0.1 % BW)

angle integrated photon spectral flux (undulator, beam intensity)



PETRA IV project

- Design group started beginning 2016
- Many groups from M/FS have been now involved, project structure starting to crystallize
- Extensive work on the "physics case" has been performed
- Significant progress on the conceptual storage ring and injector complex design achieved (subject of this talk)
- DESY management/PR actively work on securing funding
- Work of many people



Historical development – synchrotron light source lattices

Sands, Physics of electron storage rings (1970). Further developed SR theory due to Schwinger and others to show

$$\epsilon_{x} = \frac{C_{q}}{j_{x}} \left(\frac{E}{m_{0}c^{2}}\right)^{2} \frac{I_{5}}{I_{2}} \quad I_{2} = \int ds \frac{1}{\rho^{2}} \quad I_{5} = \int ds \frac{\mathcal{H}}{|\rho|^{3}} \quad \mathcal{H} = \frac{1 + \alpha_{x}^{2}}{\beta_{x}} D_{x}^{2} + 2\alpha_{x} D_{x} D_{x}' + \beta_{x} D_{x}'^{2}$$

First lattice optimized for light sources: NSLS DBA (Chasman, Green, 1975). See also Panofsky, Steffen 1960s

Petra III is a hybrid between a light source DBA and a FODO lattice used in colliders





Widely used in 3rd gen. sources



Lattice design: TME

- Applications for emittance minimization: light sources, linear collider damping rings
- Emittance minimization problem in an isolated optical cell could be rigorously solved
- θ³ dep. on bending angle for all cell types: more magnets and shorter cell length
- Modified TME with combined-function dipoles
- Real machine: TME-ish + matching for ID



$$\varepsilon = \frac{C_q \gamma^2 \theta^3}{12\sqrt{15}J_x} \quad C_q = 3.83 \times 10^{-13} m^{-1}$$

$$\beta^{\star} = \frac{L_B}{2\sqrt{15}} \quad \alpha^{\star} = 0 \quad D^{\star} = \frac{L_B^2}{24\rho} \quad \mu^{\star} = 142^0$$



L.C Teng Minimizing the Emittance in Designing the Lattice of an Electron storage Ring, Fermilab Report No TM-1269 (1984) P. Emma and T. Raubenheimer, Systematic approach to damping ring design, PRST AB 4, 021001 (2001) Y. Jiao, Y. Cai and A. Chao, "Modified theoretical emittance lattice for an electron storage ring...", PRST AB 14, 054002 (2011 Ilya Agapov | Petra IV | DESY Accelerator Physics Seminar | Page 9

Nonlinear dynamics

- Pushing down emittance by stronger focusing leads to complications with non-linear dynamics
- Hamiltonian of particle motion

in Frenet-Serret coordinates

$$\mathcal{H} = e\phi + c\sqrt{m^2c^2 + \left(\mathbf{p} - e\mathbf{A}/c\right)^2}$$

$$\mathcal{H} = -\frac{eA_s}{c} - \left(1 + \frac{x}{\rho}\right)\sqrt{\frac{E^2}{c^2} - m^2c^2 - p_x^2 - p_y^2}$$

Mag. field multipoles



Approximate Hamiltonian with multipole field expansion up to 3rd order

$$A_s \frac{e}{p_0 c} = -\frac{x}{\rho} - K_x \frac{x^2}{2} - K_1 \frac{y^2}{2} + \frac{S(s)}{6} (x^3 - 3xy^2)$$

$$B_0(s) = \frac{p_0 c}{e\rho(s)} \qquad K_1(s) = \frac{eB_1(s)}{p_0 c} = \frac{e}{p_0 c} \frac{\partial B_y}{\partial x} \qquad K_x = K_1 - \frac{1}{\rho^2} \qquad S(s) = \frac{e}{p_0 c} \frac{\partial^2 B}{\partial x^2} \qquad \Delta = \frac{p - p_0}{p_0 c}$$

$$\mathcal{H} = \frac{p_x^2}{2} + \frac{p_y^2}{2} - \Delta \frac{x}{\rho} + (1 - \Delta) \left[-K_x \frac{x^2}{2} + K_1 \frac{y^2}{2} \right] + (1 - \Delta) \frac{S(s)}{6} (x^3 - 3xy^2)$$



Sextupole field necessary to compensate energy dependence of focusing (chromaticity)
 Chromaticity and its compensation (S) and thus nonlinearity grow with lattice focusing strength (K)

Nonlinear dynamics

Linear part of the motion is solvable (Courant-Snyder parametrization)

$$\mathcal{H} = \frac{p^2}{2} + \frac{K(s)z^2}{2} \qquad z(s) = a\sqrt{\beta(s)}\cos(\eta\phi(s) + \delta)$$

Transformation to action-angle variables – solvable motion

$$z = \sqrt{2J\beta(s)}\cos\psi \qquad p = -\sqrt{2J/\beta(s)}\left(\sin\psi - \frac{\beta'(s)}{2}\cos\psi\right) \qquad J = \frac{1}{2\beta(s)}\left[z^2 + \left(\beta(s)z' - \frac{\beta'(s)z}{2}\right)^2\right]$$
$$\mathcal{H} = J/\beta(s) \qquad J = const \qquad \psi(s) = \psi(0) + \int_0^s \frac{ds'}{\beta(s')} \qquad unstable$$
Hamiltonian in action-angle variables – isolating nonlinearity
$$\mathcal{H} = \frac{1}{2}(p^2 + K(s)z^2) + \frac{S(s)}{6}z^3 \qquad \mathcal{H} = J/\beta(s) + \frac{\sqrt{2}}{3}S(s)(J\beta(s))^{\frac{3}{2}}\cos^3\psi$$
Linear frequency $\sim \cos(3\psi)$

Geometrically: unstable (hyperbolic) fixed points in phase space limit stability region, whose size is proportional to the distance from resonance

Perturbation does not average out when linear frequency is resonant $\mathbf{m} \cdot \mathbf{\nu} = n$ (in the above case m=3) Ilya Agapov | Petra IV | DESY Accelerator Physics Seminar | Page 11

Resonances and a toy model of Henon-Heiles-type

Hénon, M.; Heiles, C. (1964). "The applicability of the third integral of motion: Some numerical experiments". The Astronomical Journal. 69: 73–79.

Generic Hamiltonian at isolated resonance

No frequency change with amplitude – resonance (linearly) unstable Frequency changes with amplitude – many resonances driven Resonance islands overlap – chaos. Chirikov criteria for island separation

$$\mathcal{H} = \nu J + \alpha(J) + f(J)\cos(m\psi - n\theta)$$

$$\sqrt{\alpha^{\prime\prime}(J_r)f(J_r)}\ll \frac{\Delta\nu}{4}$$

"Detuning times driving smaller than resonance distance"

Dynamics with sextupole nonlinearity similar to Hénon-Heiles which was often used as a toy model: M_{SEXT} o M_{LIN}



Could be easily seen that $M_{SFXT} \circ M_{UN} \circ M_{SFXT}$ with linear phase advance of π , 3π , etc. has no nonlinear terms: -/ transform between sextupoles an effective nonlinear cancellation strategy Ilya Agapov | Petra IV | DESY Accelerator Physics Seminar | Page 12

Real machines: detuning and resonance crossing



Petra III lattice, if the tune moved close to 1/3 resonance DA limitations



MBA lattice – nonlinear momentum detuning

Could design a lattice which does not drive high order resonances. Half integer typically hard to cross







Lattice design: MBA machines

- MBA machine proposals emerging in 1990s (Einfeld et al.)
- Pioneering implementation with MAX IV. A number of 3GeV designs followed (e.g. Sirius)
- PEP-X and tau-USR conceptual studies for sub 10 pm machines in US discontinued
- 'Hybrid MBA' lattice from ESRF-EBS the lattice of choice for 4th generation rings. Relies on close to –I transformation between sextupoles



Lattice design specifics for Petra IV

- Several MBA lattice types can deliver natural (bare) emittances in the 10 pm range at 6 GeV with PETRA geometry
- At the same time, dynamic aperture required for accumulation (5-10 mm for PETRA IV) and safe beam manipulation is hard to achieve
- The PETRA geometry (long straights, low degree of symmetry) presents opportunities
 - Optimized cell design for arcs with no IDs
 - Non-local chromaticity correction schemes
 - Very long insertion devices
 - Damping wigglers
- ...as well as difficulties
 - Large DA is generally harder to achieve in asymmetric rings
 - Long straights create extra aberrations
 - More effort for optics design (more magnet families, more matching etc.) in general compared to more conventional SR sources





Putting (nearly) everything together - USR





- R. Brinkmann Beschleuniger Ideenmarkt 2015, first considerations on the possible PETRA IV lattice
- Two phase space exchanges in the ring (similarity to Möbius scheme, but optics is always in one mode locally)
- Nonlinear cancellation with –I phase advance between sextupoles
- Phase space exchange allows one sextupole family only
- Sum chromaticity is corrected only, local chromaticity can be substantial

$$\xi_x^A + \xi_y^B = 0 \quad \xi_y^A + \xi_x^B = 0$$





Optics built on this principle



"no-ID" octant



6BA undulator cell

6BA "empty" ("no-ID") octant cell



Half ring coupled optical functions





- Phase space exchange not a limitation
- Distributed chromaticity correction a mild limitation (large local chromaticity)
- I sextupoles yield excellent transverse dynamics, but need to optimize off-momentum dynamics (2nd and 3rd order chromaticities)
- The number of knobs for off-momentum dynamics optimization is limited (redistribution of sextupole strength between arcs)
- Strong energy spread damping by undulators due to partition shift

$$\left(\frac{\sigma_{E,wig}}{\sigma_{E,0}}\right)^2 = \frac{1 + \frac{\mathcal{I}_{3,wig}}{\mathcal{I}_{3,0}}}{1 + \frac{\mathcal{I}_{2,wig}}{\mathcal{I}_{2,0}}} \frac{j_{z,0}}{j_{z,wig}}$$

Parameter	Value
Beam energy	$6 \mathrm{GeV}$
Emittance, bare lattice (hor., vert.)	$28~\mathrm{pm},28~\mathrm{pm}$
Emittance, 0.7T (rms) IDs	$12~\mathrm{pm},12~\mathrm{pm}$
Energy spread, bare lattice	$2.6 \cdot 10^{-3}$
Energy spread, 0.7T IDs	$1.0 \cdot 10^{-3}$
Integer tunes	123, 123
Natural chromaticity	-188 , -188



Influence of the phase space exchange on the 3rd order resonance structure (simplified lattice model)



- Low degree of symmetry could be partially offset by arc achromats and chromaticity redistribution to yield acceptable MA
- Large DA limited by synchro-betatron coupling and path lengthening effect $\Delta C = -2\pi (J_X \xi_x + J_Y \xi_y)$



I. Agapov, R. Brinkmann, J. Keil and R. Wanzenberg. Phys Rev AB 21, 051601 (2018)

N1 Round beams turned out to be not an attractive option from user perspective High Compound High resolution refractive precision Heavy P09 diffr. load diffr. HAXPES High heatload mono lenses monochromator $\theta_1 \theta_0 \theta_1$ $\Delta \theta$ Undulator λb BPM Phase retarder Exp. 2 Exp. 3 Exp. 1 θh Frontend Optics hutch Matsushita http://cheiron2010.spring8.or.jp/

Lattice design: HMBA lattice

- Same cell of ESRF-EBS type in octants
- ESRF-EBS achieves good nonlinear aberration cancellation with relatively simple due to the –I rule for hor. sextupoles
- Pursued in parallel with T lattice





Parameter	PETRA III	PETRA IV	PETRA IV
		(without DW)	(with DW)
Energy / GeV	6	6	6
Total current / mA	100	100	100
Nat. emittance ϵ_0 / pm	1280	15	9.3
Energy spread $\sigma_p / 10^{-3}$	1.23	0.73	1.44
Energy loss/turn U_0 / MeV	5.1	1.37	4.6
Momentum compaction	1.13	0.0146	0.0146
factor $\alpha_c / 10^{-3}$			
Dispersion at SF D_x / cm	750	4.2	4.2

Parameters of PETRA III / IV without intrabeam scattering.

Two ring octants with the injection section



Lattice design: HMBA lattice

- Initial lattice implementation with ESRF-EBS cell had DA/MA problems
- Issues addressed:
 - proper length and magnet strength scaling to achieve theoretical DA scaling from the original ESRF-EBS $(A \sim (\rho_1 / \rho_2)^2)$
 - Give up 23m cell length
 - 4th order geometric achromat condition in arcs
- Current reference lattice (included extensions, canting etc.)
- Open issues:
 - Small optics "insertions" perturb nonlinear dynamics
 - Alignment errors will reduce the DA. Extent tbd.





Lattice design: DMI lattice

- A non-interleaved lattice, but beam shape is not limited to round
- Chromaticity correction mostly in the "no-ID" arcs with special cells, 2 cell types
- Full ~20pm lattice assembled (with extensions). Good DA (>15 mm) but MA is limited
- Relies on PETRA geometry with most of the ring w/o IDs



D(m)



Tolerances

- Element misalignments in the few µm range can already lead to an unstable machine. Mechanical stabilization important
- This is due to a large amplification factor. Optics unstable when orbit is in hundreds of µm range. BPM resolution in 1 µm range should be theoretically sufficient for BBA. Detailed studies in progress
- Results from APS and ESRF studies and first simulations suggest that alignment of 100 µm girder + 30 µm on girder with BPM resolution of 30 µm shot-to shot an 0.1 µm orbit might be sufficient
- Impact on DA and emittance might be however different from APS or ESRF
- Under investigation, simulations in progress



Closed orbit existence vs. misalignment

Closed orbit existence vs. misalignment in a "feedback simulation"



Girder design collaboration MEA/AWI Bremerhaven



20μm girder + 3μm on girder 1Similar effect in PETRA III with 100μm- 200μm



Closed orbit existence limit PETRA III w/o orbit correction ~1.1 mm

Collective effects

- IBS limits the beam emittance for most operation scenarios and lattice types
- Lattices below 15 pm bare emitt. do not improve the real emittance, due to IBS limitation



Momentum acceptance of >2% required to provide beam lifetime of several hours

- Round beams (*I. Agapov et al., proc. IPAC 2018, I. Agapov and R. Brinkmann, proc. NOCE2017*) would help mitigate both IBS and Touschek and will be essential for "timing mode" (high bunch charge mode)
- Impedance-driven instabilities (e.g. TMCI) limit the bunch current to about 1mA



Target parameters – influence of undulators

- Undulators have significant impact on emittance
- Typical ID configuration gives 0.1% energy spread and 10 pm emittance (no canting, no IBS, no DW)

5.4 mrad

- Canting (depending on angle)
- 4 mrad canting for some IDs is tolerable
- Due to strong influence of the number of operating IDs and gaps, will need some feedback mechanisms to stabilize emittance in user operation

2.7 mrad

Scenario with a 25 m cell no canting with 24 mm IDs Different beta functions at ID



Scenario with a large emittance 23 m cell with 24 mm IDs Different beta functions at ID

Electron beam

X-Ray bes

PM Steerer

2.7 mrad

Canting schematic from J. Chavanne et al.

(ESRF), proc IPAC 2010





Advanced options

- Typical advanced radiation options are coherent radiation or short pulses.
- High gain FEL in a PETRA-like using local longitudinal RF compression is feasible (I. Agapov, NIM A 793, 2015) but limited to soft x-rays and technically challenging
- New take on this subject: Bragg cavity XFEL Oscillator with TGU is feasible

$$\lambda = \frac{l_w}{2\gamma^2} \left(1 + \frac{K(x_\beta + \eta\sigma_\eta)^2}{2} \right)$$

$G \sim \frac{1.53\pi^3 \gamma \lambda}{\gamma}$	$K^2[JJ]^2$	N_w/σ_η
$0 \sim \frac{l_w}{l_w}$	$1 + K^2/2$	$\overline{D/\sigma_x + (5.46N_w)^2 \sigma_x/D}$

Long	inse	rtion
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I. Agapov et al. proc IPAC 2018

Collaboration with ANL









OCELOT

- Software tools used in optics design: *madx, ptc, opa, elegant, at, lego, ocelot*
- OCELOT started in 2011 as a C++ beam dynamics framework with a wakefield focus (Agapov and Zagorodnov KWT Seminar 2011), completely rewritten in python for XFEL.EU SR/FEL simulation purposes (Agapov et al. Proc IPAC13 Shanghai), implemented comprehensive beam dynamics capabilities (I. Agapov et al., NIM A 768 2014)
- Mostly used for linac and FEL simulations
- Physics: beam transport up to 2nd order or drift-kick-drift, CSR, wakefields, space charge, Ming Xie FEL estimator, genesis interface, x-ray optics, SR radiation
- Includes advanced on-line control and optimization module
- Open source "community project" <u>https://github.com/ocelot-collab</u> current lead developer
 S. Tomin (since 2016). Web-based tutorials to get started

European XFEL linac





OCELOT optimization

Started as FLASH accelerator R&D in 2015. Now a suite of tools widely used at XFEL.EU, LCLS and FLASH. Partially ported to PETRA (generic optimizer: configured for linac transmission efficiency). Collaboration with SLAC/LCLS.



Orbit correction



I. Agapov et al. proc IPAC 2015 S. Tomin, I. Agapov et al.,, proc IPAC 2016 I. Agapov et al., proc. ICALEPCS 2017 I. Agapov et al., DESY-17-054 I. Agapov et al. proc IPAC 2018

Generic optimizer





Orbit adviser



Machine Learning

- ML is essentially a way of programming: generic tools fed with training data instead of "algorithms".
- Theory long known (backpropagation algorithm for deep NN training introduced somewhere between 1970 and 1983) but ubiquitous data (essential for such methods) is a recent phenomenon
- Many strong players in industry and government (e.g. 2017 DoD AI budget \$7.4 B <u>https://www.wsj.com/articles/the-new-arms-race-in-ai-1520009261</u>)
- Socio-economic and ethical challenges to be addressed <u>https://techcrunch.com/2018/06/14/here-are-the-experts-who-will-help-shape-europes-ai-policy/</u>
- Growing body of AI-inspired physics research: Titles from recent PRL vol 120 issue 24:

Machine Learning Detection of Bell Nonlocality in Quantum Many-Body Systems; Experimental Machine Learning of Quantum States; Exploring the Function Space of Deep-Learning Machines

- Accelerator controls is probably most similar to autonomous driving. However the problem statement very different. Learning material for supervised learning scarce. Research needed. Synergies essential.
- ML activities in accelerators (see e.g. APS BP newsletter https://www.aps.org/units/dpb/newsletters/upload/fall17.pdf)
 - International collaboration (also ICFA-sponsored), New workshop series "Machine Learning Applications for Particle Accelerators" https://conf.slac.stanford.edu/icfa-ml-2018/
 - In the framework of Helmholtz Incubator on Machine Learning ("HAICU", being set up)
 - In the framework of CDCS and Helmholtz DMA Programme (being set up)



ML for PETRA

- Ambitious goal: autonomous operation
- We can technically do it! But: expensive, and doing this with one facility/device won't change much. Only makes sense in the context of a larger autonomous research operation (beamlines, sample shipment etc.)
- Challenge of PETRA IV is expected complexity of machine commissioning and startup due to increased optics sensitivity
- Scaled-down goal: fast and possibly autonomous machine startup and optics correction
- Still need to reshuffle most of the HL controls
- Single-bunch single-turn diagnostics provides lots of data (to be fed into ML methods).
 Optics inference from trajectory data is potentially "instantaneous" but many effects have to be deconvolved (noise, decoherence, etc.) to yield good results
- Part of "commissioning simulations"
- Started prototyping. Proper developments should begin in parallel with TDR
- Collaboration with SLAC/SPEAR3

I. Agapov et al. proc IPAC 2018



Conclusion and outlook

- 2+ years of design converging on a viable solution
- Target emittance parameters reachable. PETRA IV could be the brightness record holder among 4th generation rings
- Technical subsystems (magnets, vacuum, mechanical stabilization, RF) challenging but requirements not beyond state of the art
- A critical issue to be addressed urgently: mechanical and thermal stabilization and dealing with alignment tolerances and high sensitivity of the lattice in general
- Difficulty in operation and machine set-up expected. Investment in automation essential
- Exciting phase ahead

