A Cavity Based X-ray FEL Demonstrator at the European XFEL

MDI technisches Forum
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Patrick Rauer on behalf of the XFELO team

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A Cavity Based X-ray FEL Demonstrator for the European XFEL

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European XFEL

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A Cavity Based X-ray FEL Demonstrator for the European XFEL

Structure

- Motivation and background
- A walkthrough
- A proof of principal experiment at the SASE1 beamline
  - Conceptual design
  - Nominal performance
  - Impact of error sources
  - The impact of heat load
- Challenges → Alignment and commissioning
- Summary

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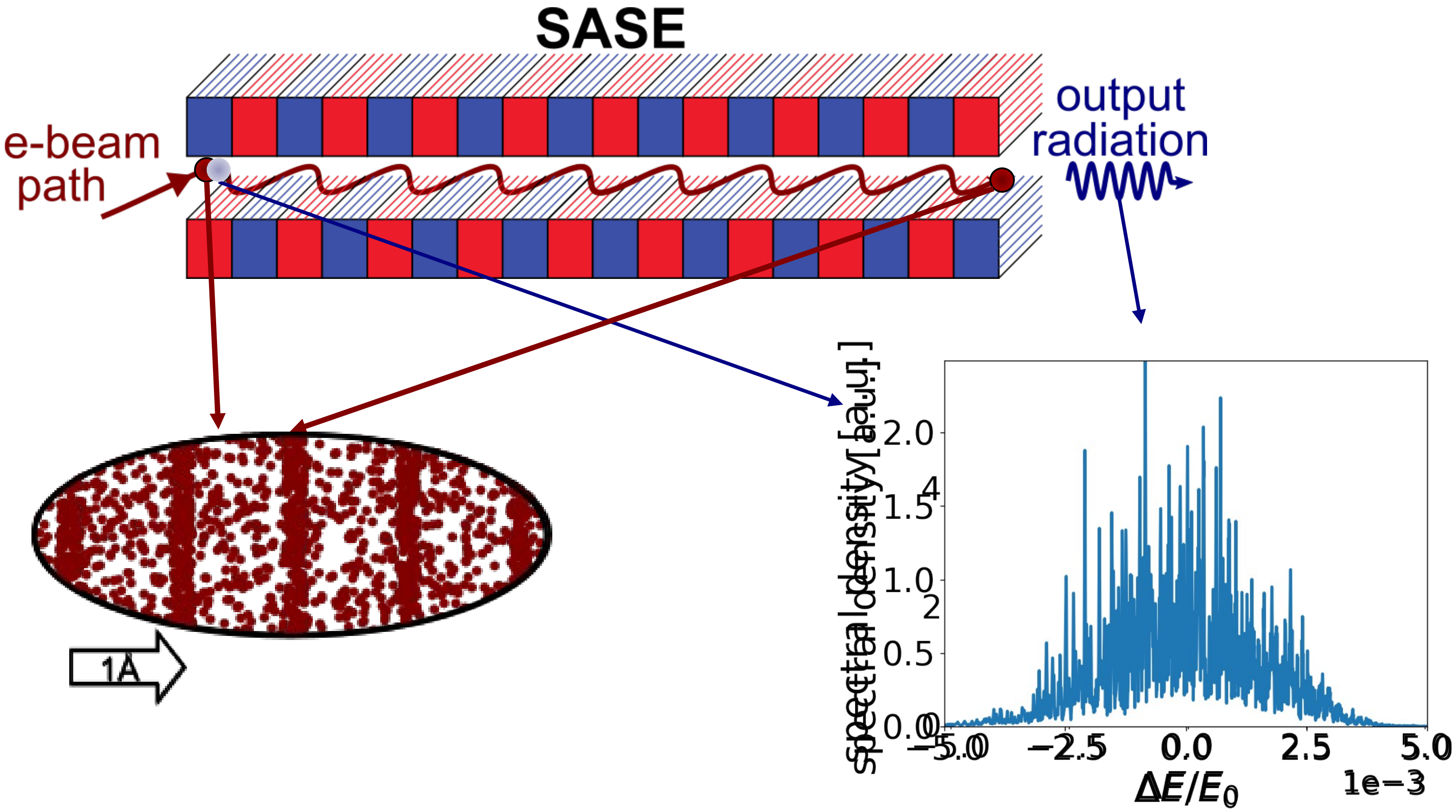
Motivation



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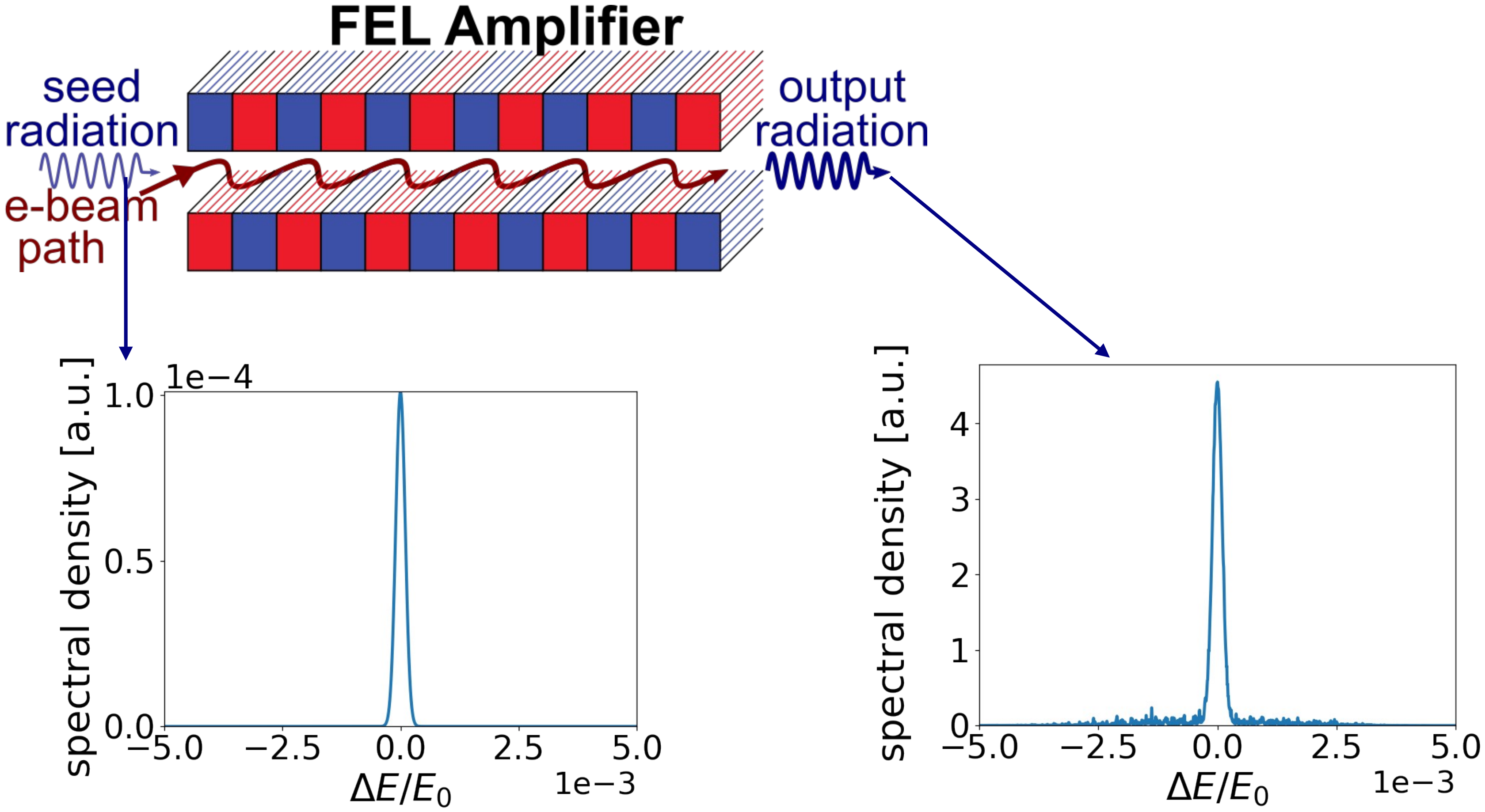
FEL-Concepts



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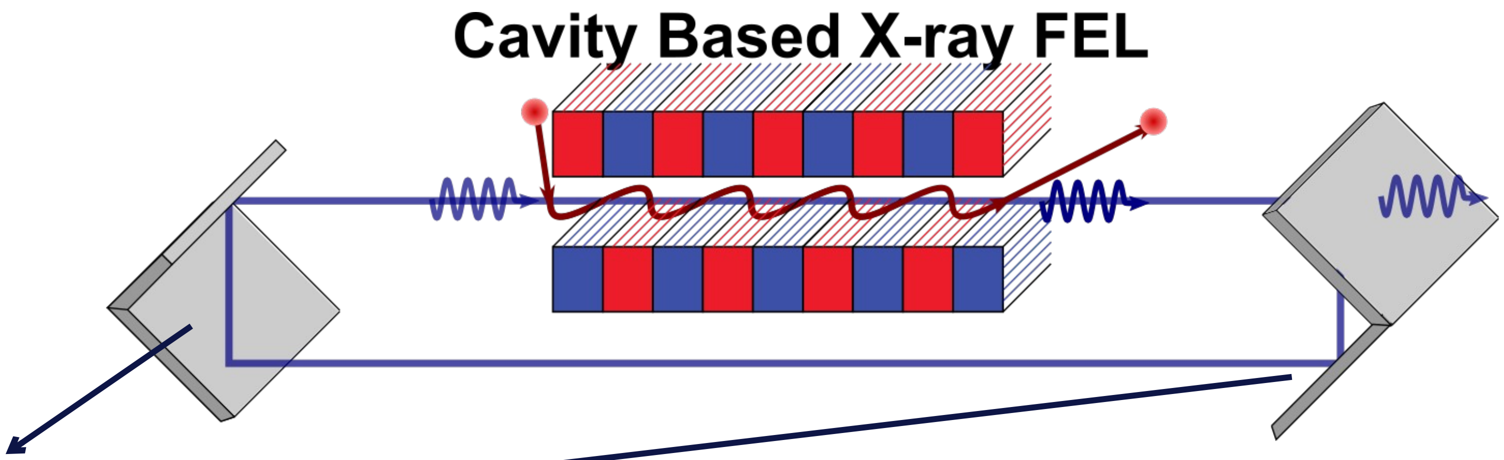
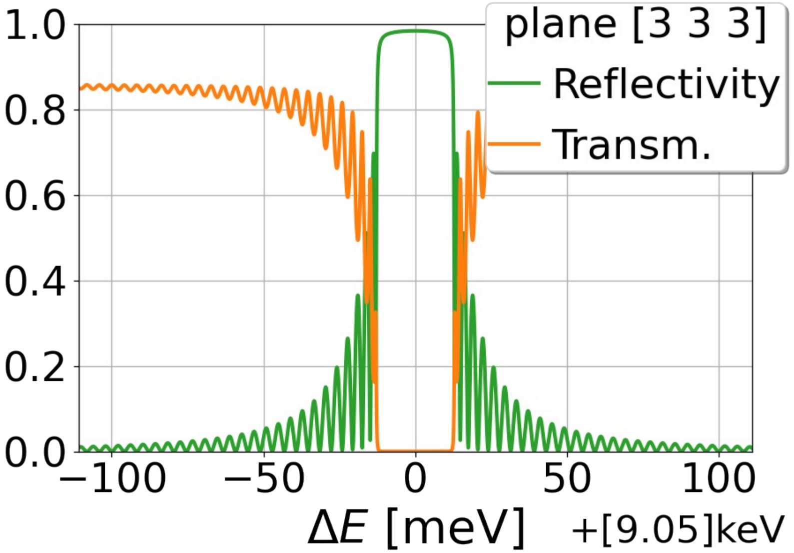
CBXFEL = X-ray cavity with monochromatizing mirrors



Bragg's law:

≊2 ·



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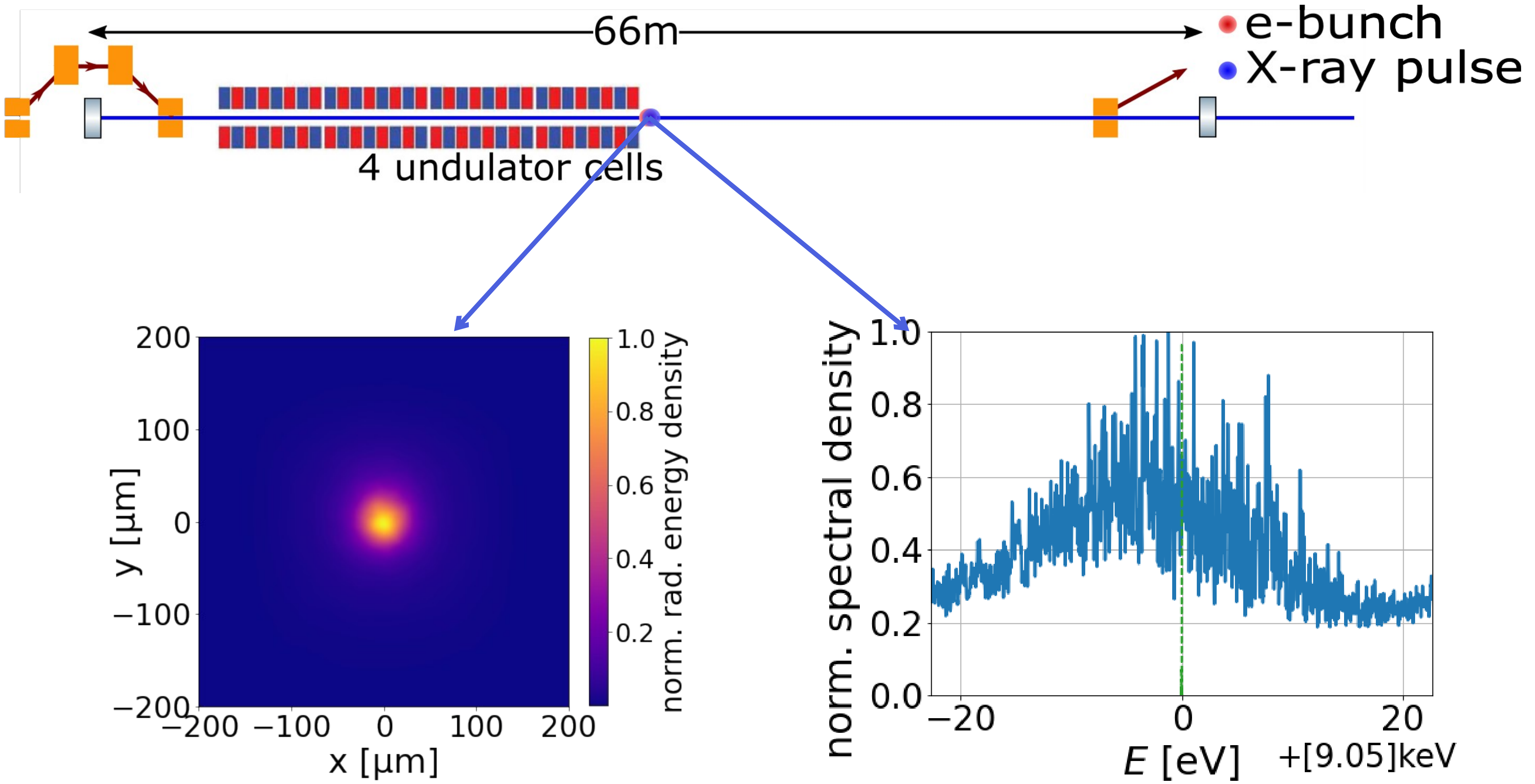
A Walkthrough



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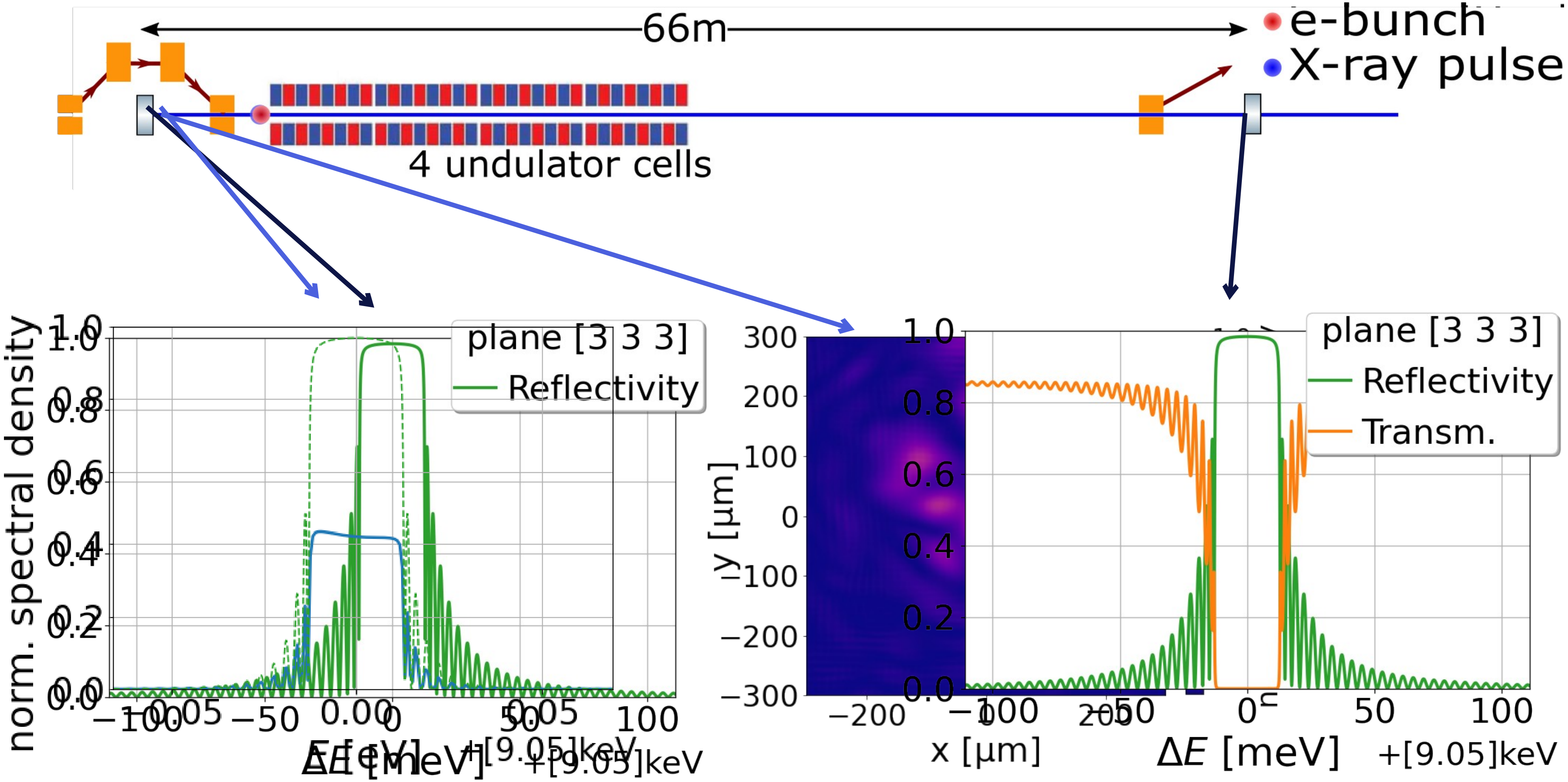
A Walkthrough



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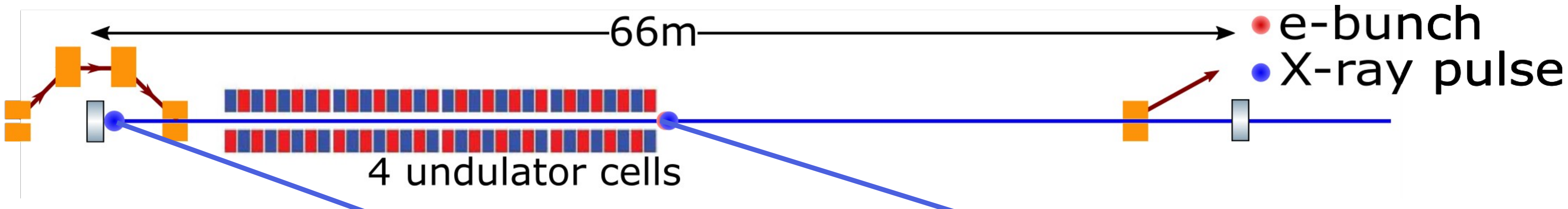
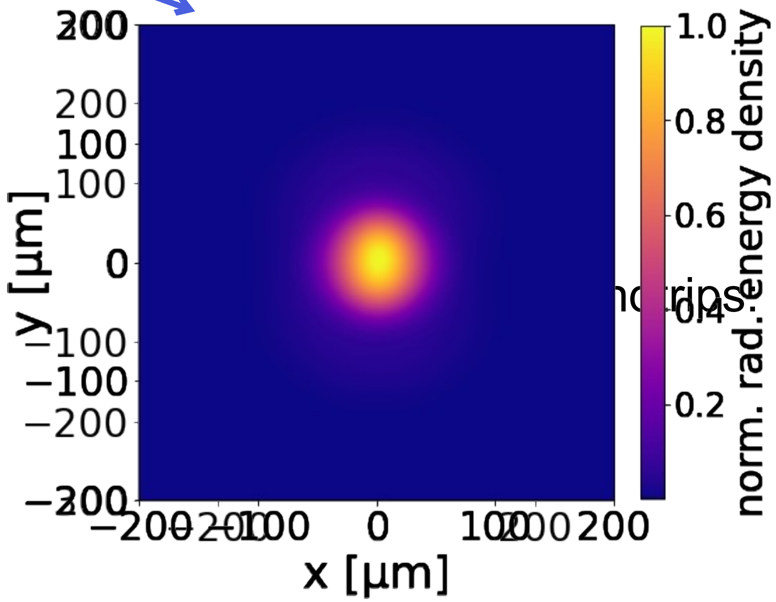
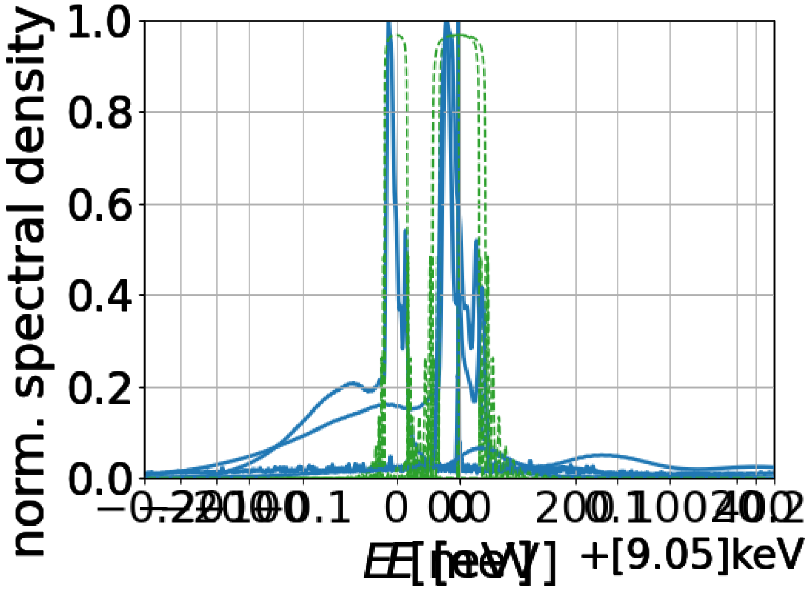
A Walkthrough



- With subsequent roundtrips:
  - Increasing coherence of FEL-radiation before refl.
  - Stabilization of transverse distributions after refl.
- **~3D coherent radiation in saturation**





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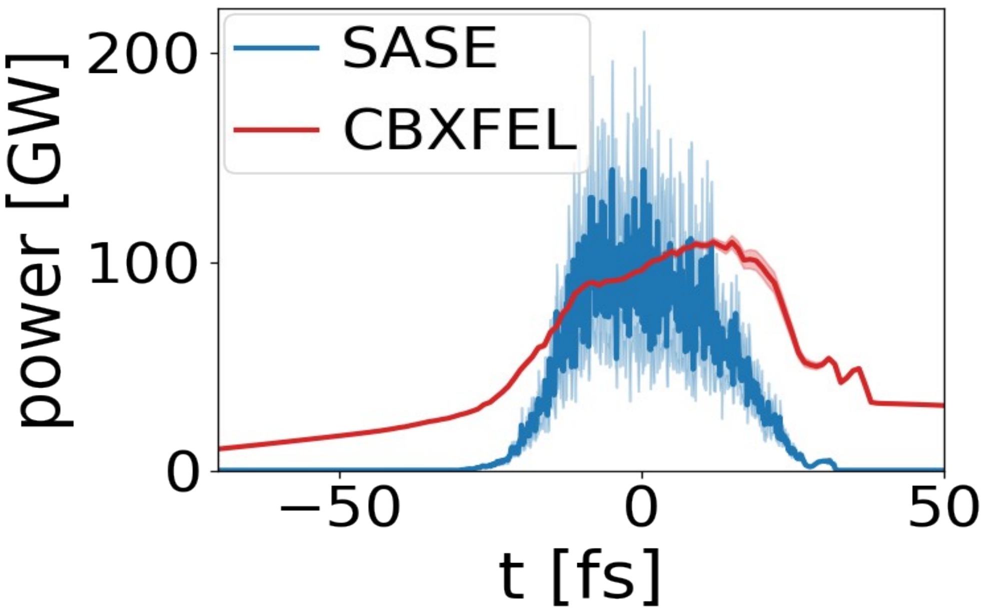
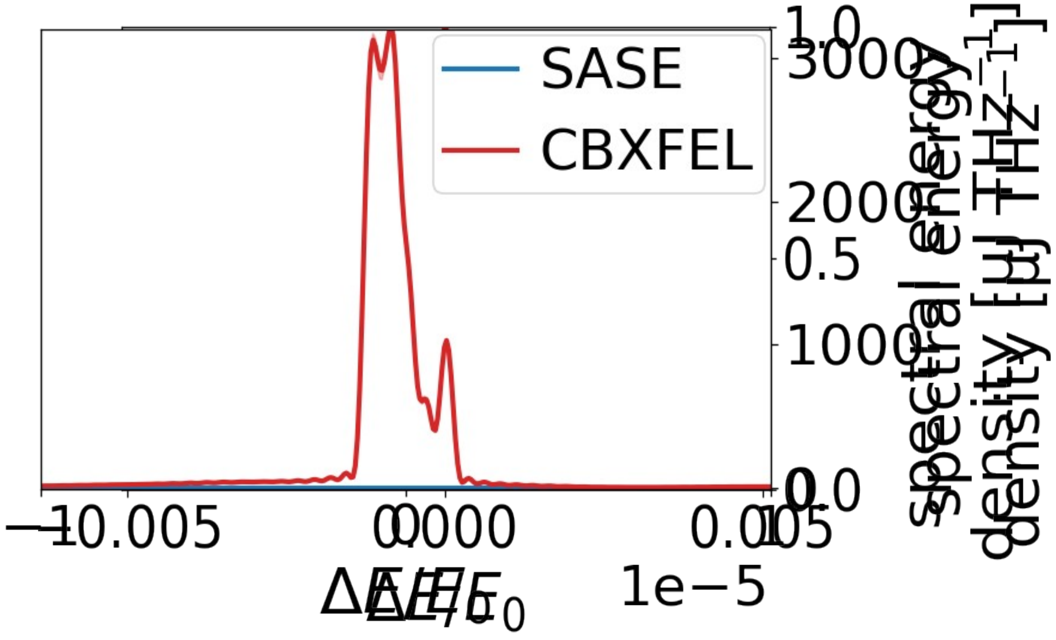
SASE vs. CBXFEL





- **CBXFEL**
  - Bandwidth
  - Very high peak spectral density
  - ~full pulse coherence (3D)

- **Use Cases**
  - Spectroscopy
  - Quantum optics
  - High peak power applications
  - Moving closer to optical lasers

    ⇒ Development potential

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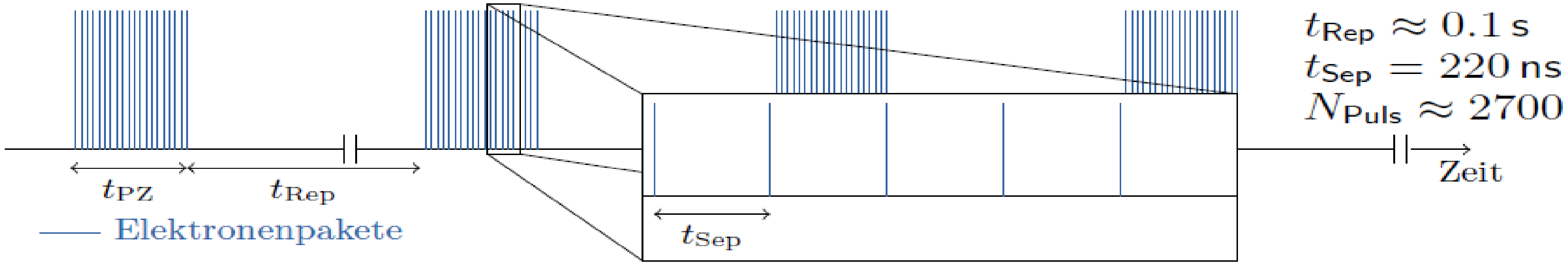
Why at the European XFEL?



- CBXFEL necessities:
  - High enough single pass gain to compensate for losses
    - ► Brilliant electron beam (Linac)
  - Matching between electron bunch repetition and photon pulse round trip time
    - ➔ In comparison EuXFEL: electron bunch repetition rate 2.25 MHz↔132 m optical path length

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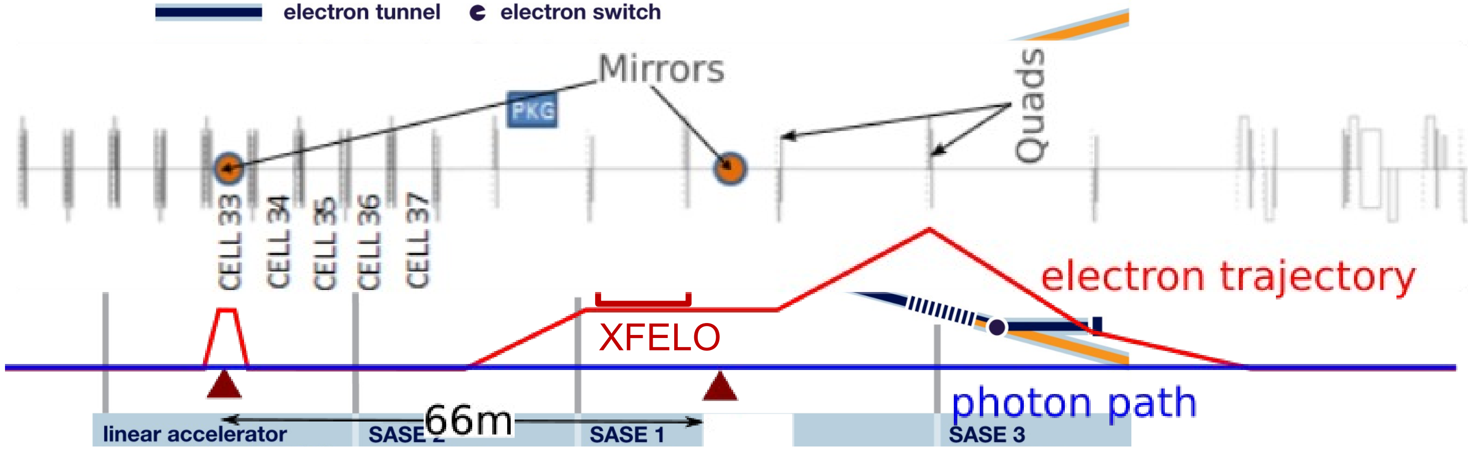
Proof of Principle Experiment at SASE1



- R&D project to realize a proof of principle CBXFEL demonstrator at the EuXFEL.
  - Located in the SASE1 tunnel
  - Using last four (typically not used) undulators
  - Based on 2.25 MHz repetition rate ↔ 132 m roundtrip length

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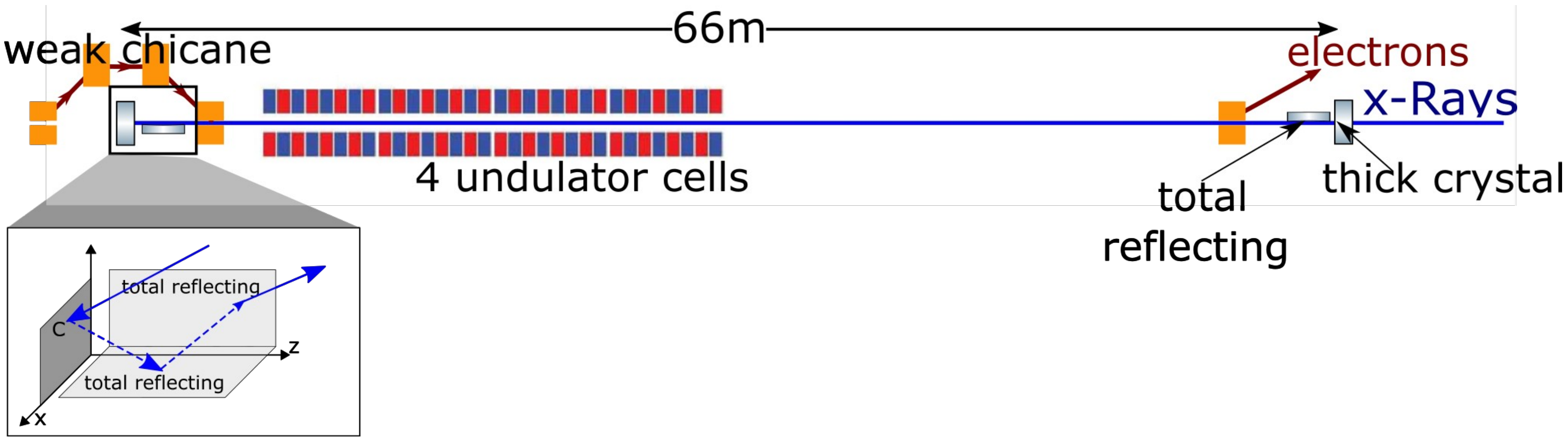
Proof of Principle Experiment at SASE1



- Principle goal: Proof that seeding (and stable operation) with a cavity based XFEL is possible!
  - Keep it simple!
    - Cavity in backscattering geometry ➔ **No wavelength tuneability**
      - ► Using grazing incidence mirrors to detune crystal some mrad from exact 90°incidence

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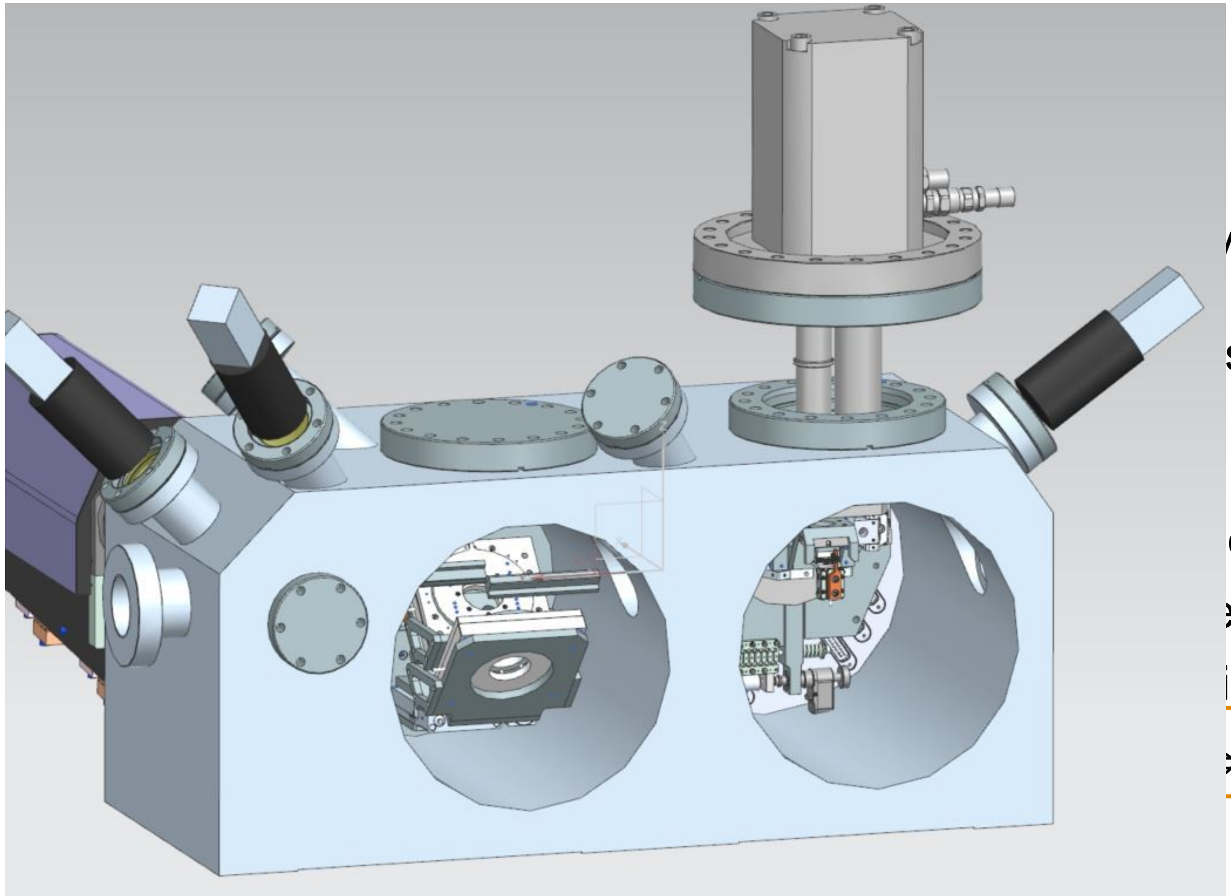
Proof of Principle Experiment at SASE1



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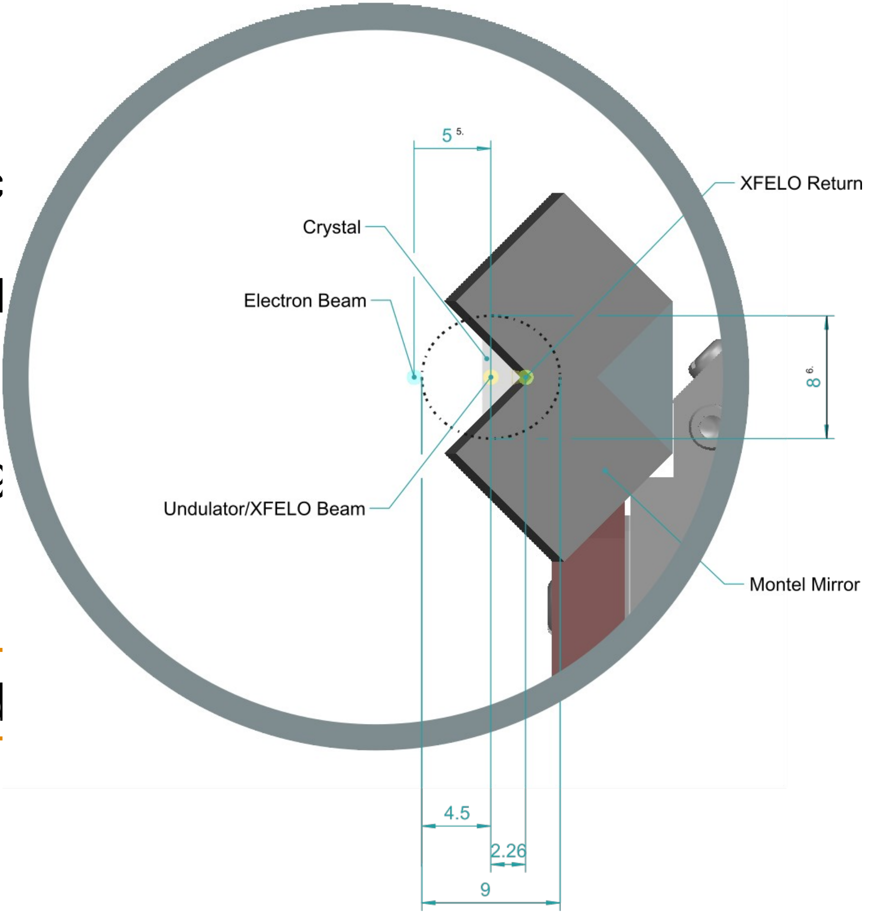
ion!

100 nrad

Retro-reflecting Monochromator2
(view from upstream to downstream)



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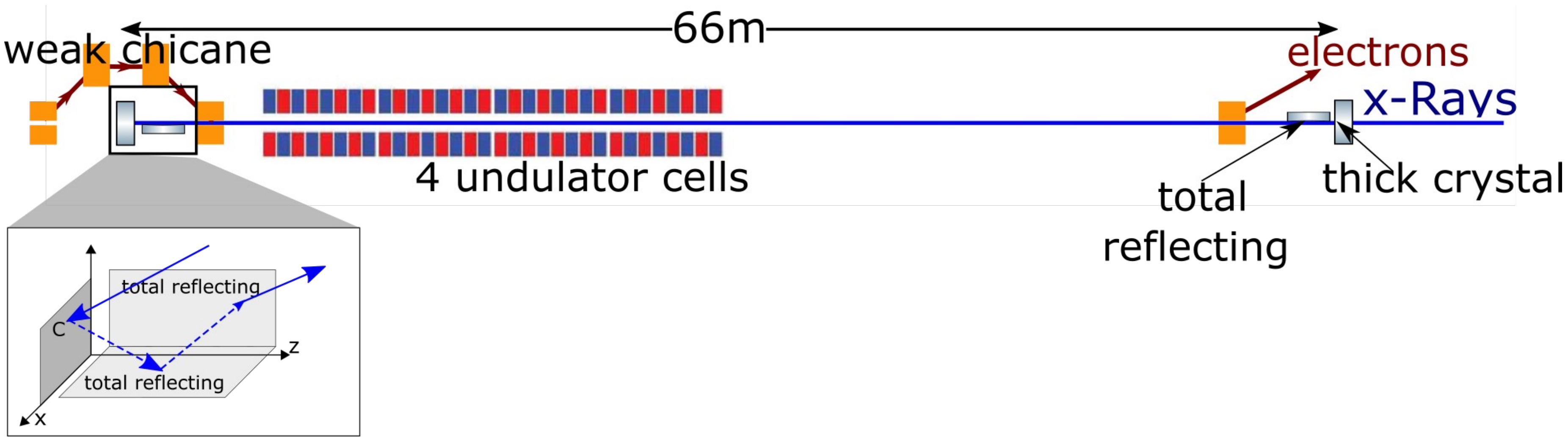
Proof of Principle Experiment at SASE1



- Principle goal: Proof that seeding (and stable operation) with a cavity based XFEL is possible!
  - Keep it simple!
    - Cavity in backscattering geometry → **No wavelength tuneability**
      - ► Using Kirkpatrick-Baez mirrors to detune crystal some mrad from exact 90°incidence
    - Shall work with regular (250 pC) SASE operation electron bunches
- Very simple transmission scheme ⇒Just use regular crystal transmission

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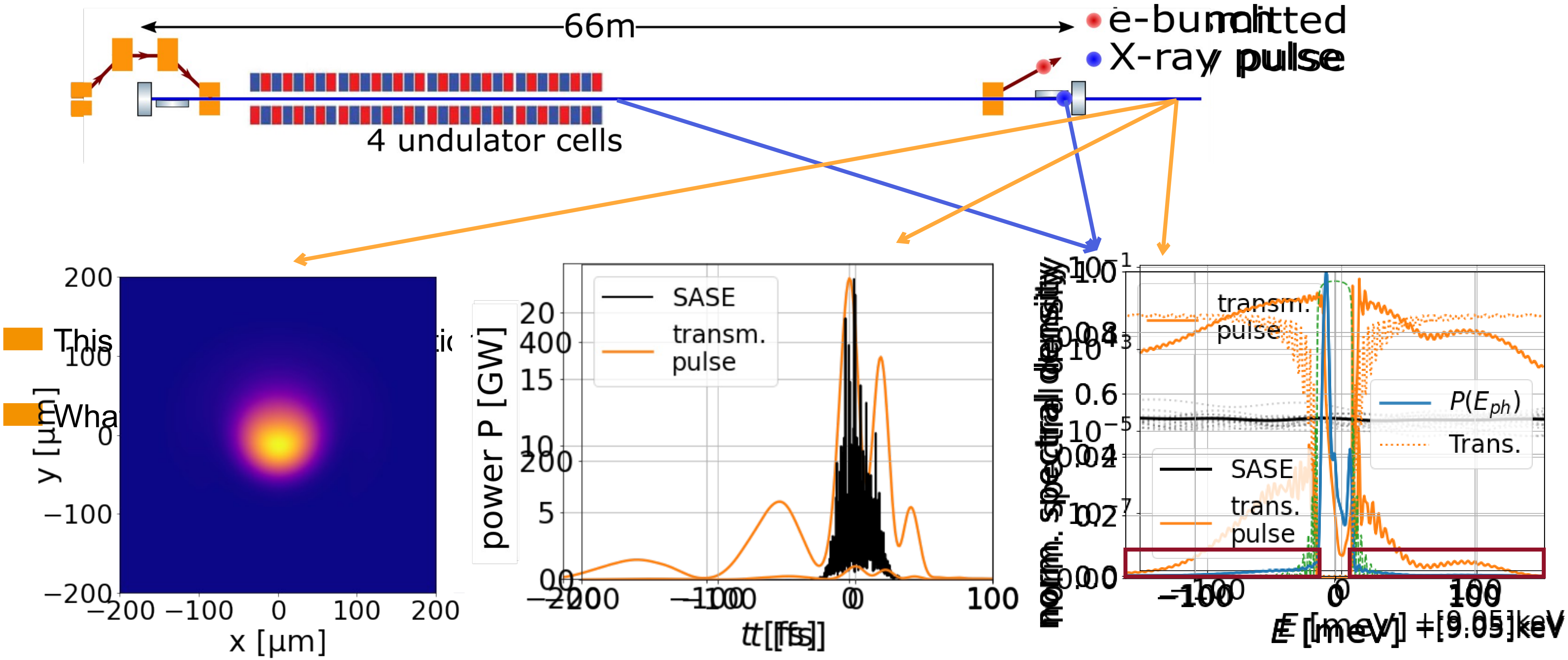
What is actually transmitted?

- This
- Wha



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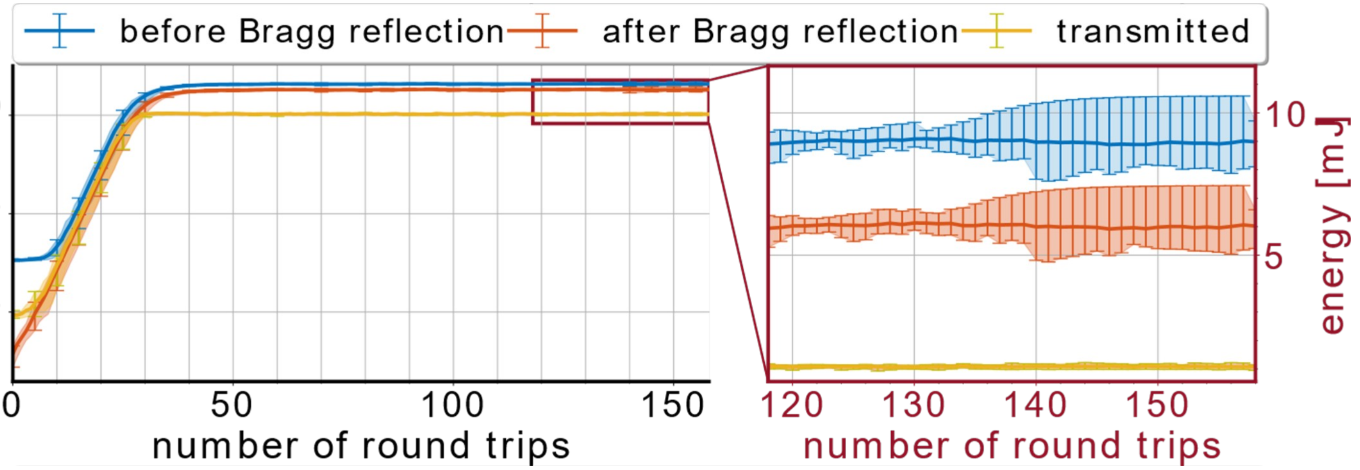
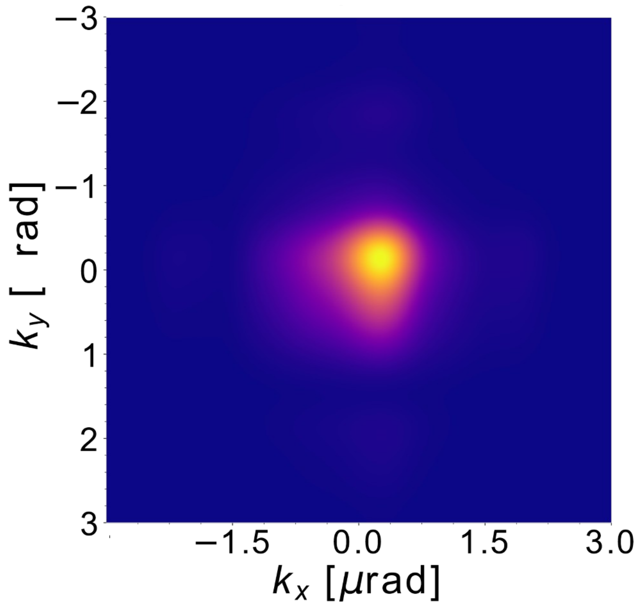
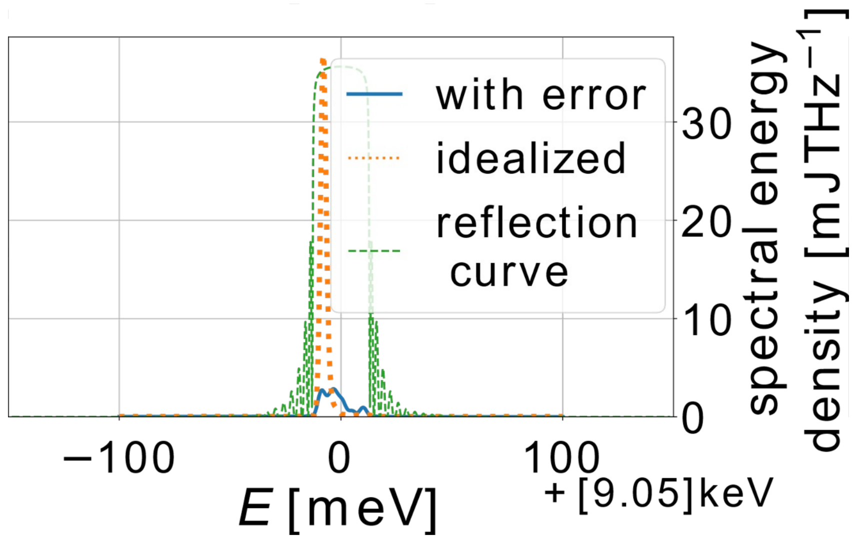
Including Alignment Error, Electron Jitter and Surface Error

$\Delta x_\perp$ [μm]	$\Delta\theta_\perp$ [nrad]	Δz [μm]
Before reflection		
10	200	10

Simulation results	
Sat. pulse energy	10.0(1) mJ
spectral width	20.4(5) meV
rms duration	132(2) fs
tf-product	4.1(2)
Brilliance	5.2(3)*10^{34}



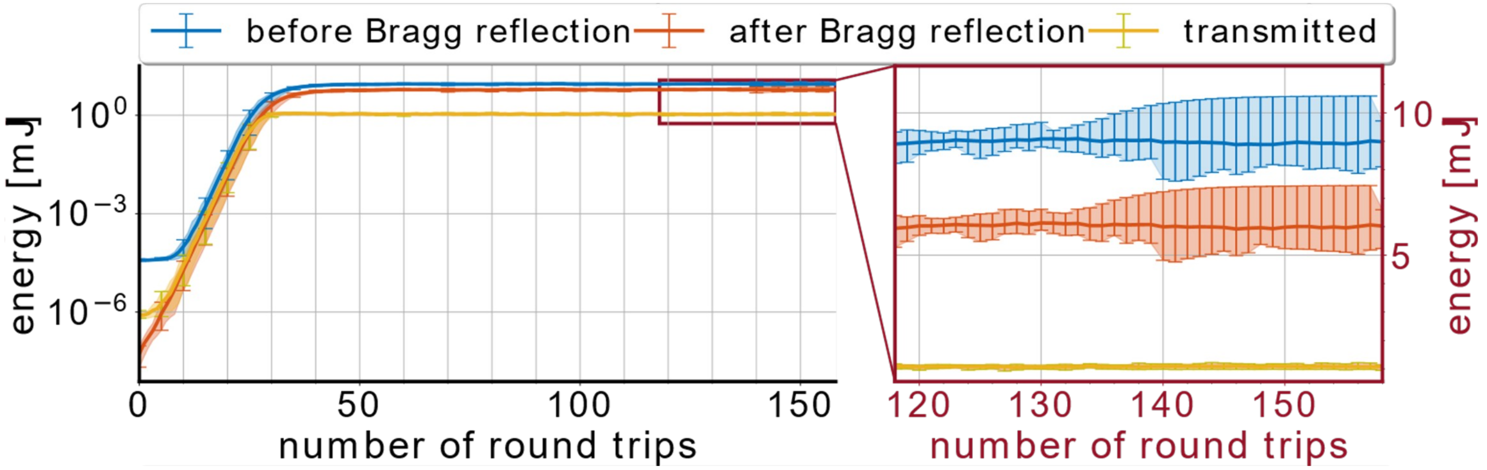


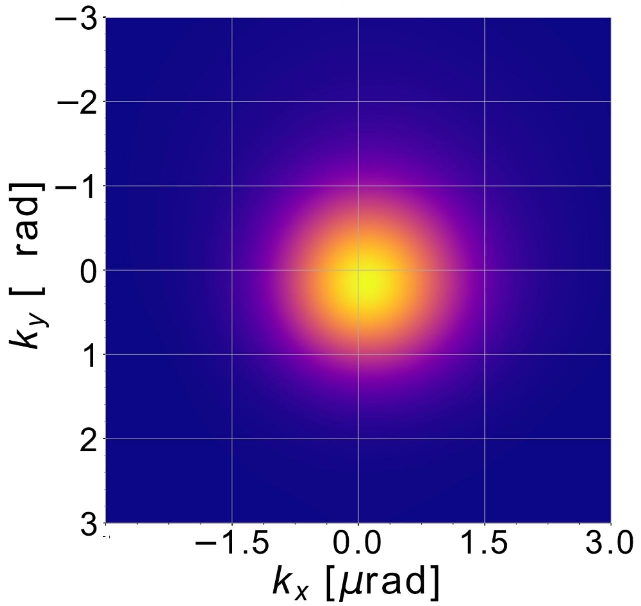


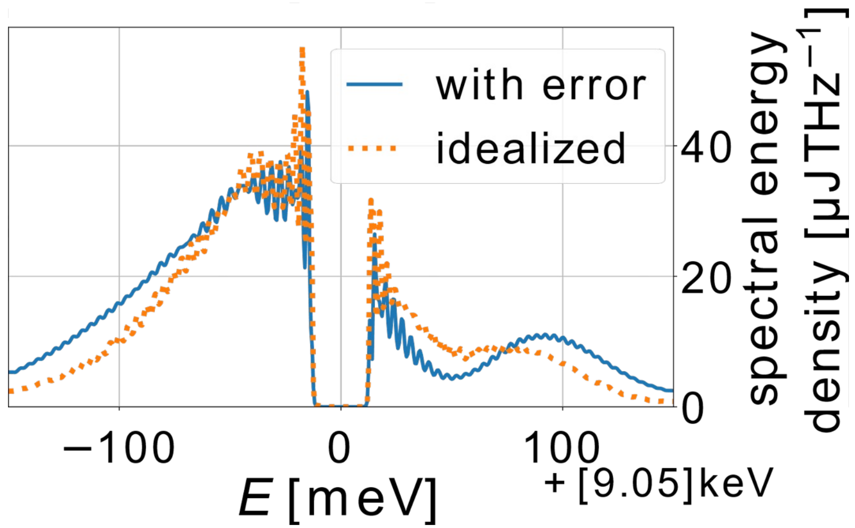
A Cavity Based X-ray FEL Demonstrator at the European XFEL

Including Alignment Error, Electron Jitter and Surface Error

Simulation results	
Before reflection	
Sat. pulse energy	10.0(1) mJ
spectral width	20.4(5) meV
rms duration	132(2) fs
tf-product	4.1(2)
Brilliance	5.2(3)*10^{34}
Transmitted	
Sat. pulse energy	0.95(5) mJ
spectral width	69(2) meV
rms duration	97(2) fs
tf-product	10.2(5)
Brilliance	1.4(2)*10^{34}







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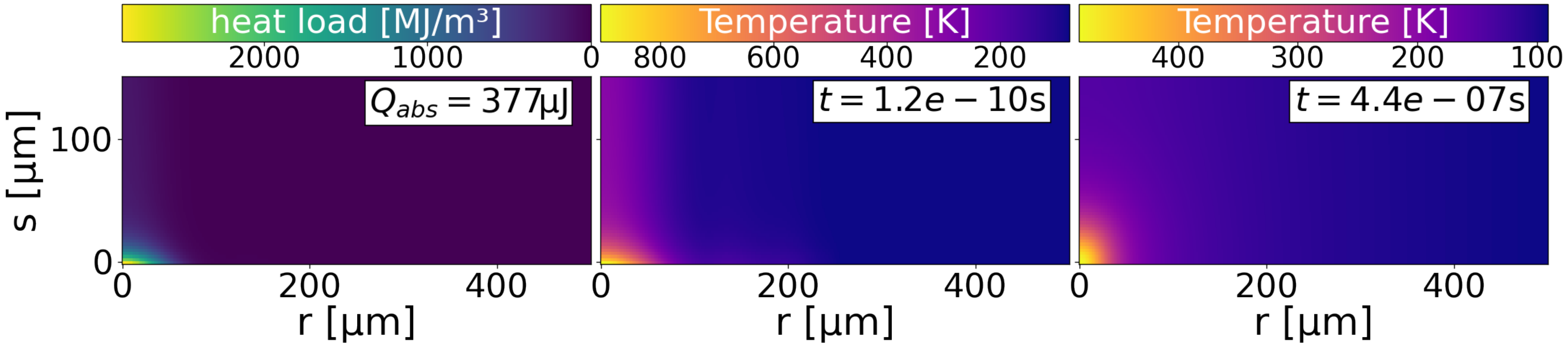
The Problem of Thermal Load: Saturated CBXFEL (~10 mJ pulse energy)



- **Heating at full pulse energy much too high**
  - Does the CBXFEL reach a stable state at lower pulse energies in fully coupled simulation?

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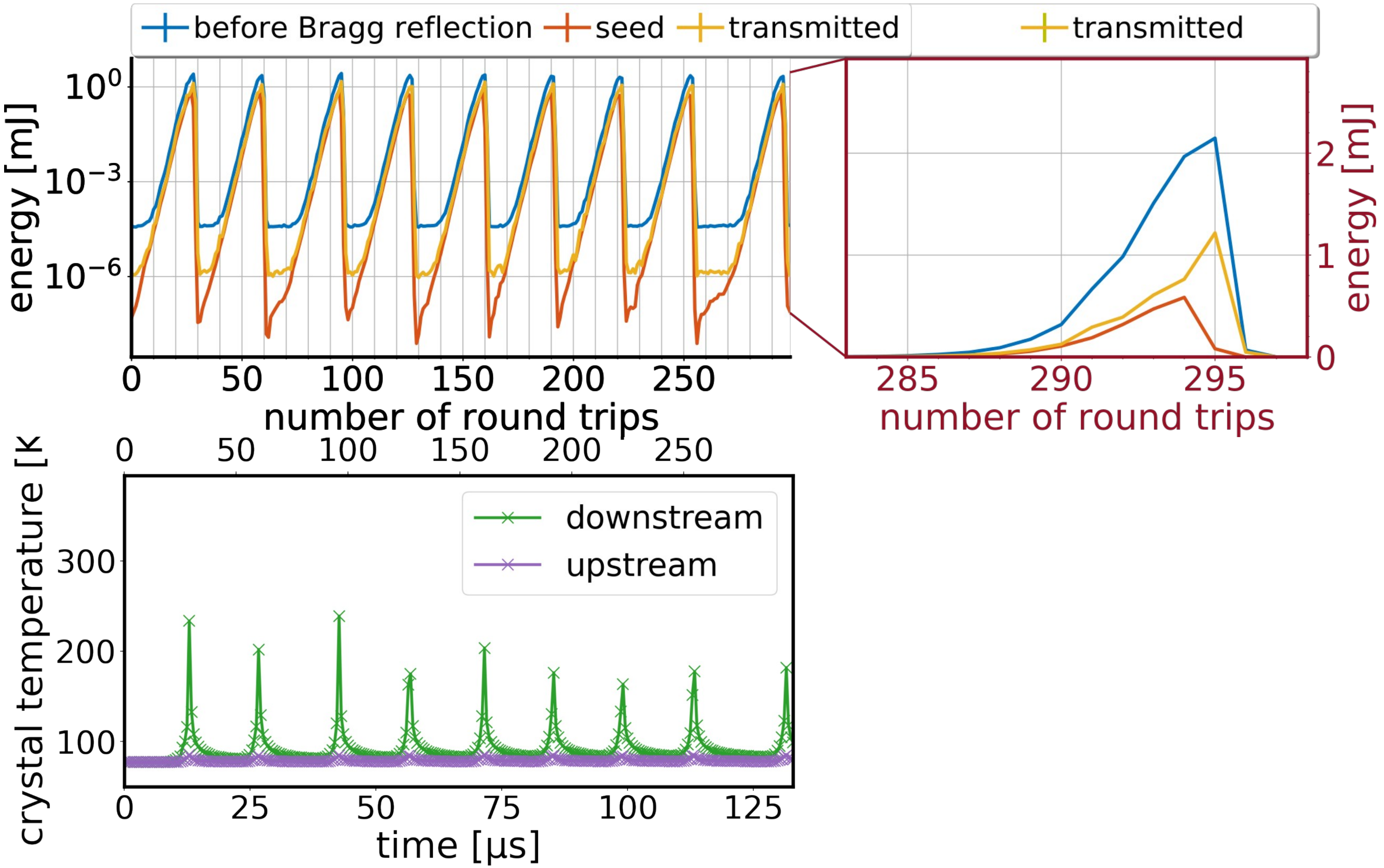
Including Thermal Response

- No stable operation
- Periodically reoccurring intense pulses
- Interesting for experimental setup
- Strongly varying pulse properties



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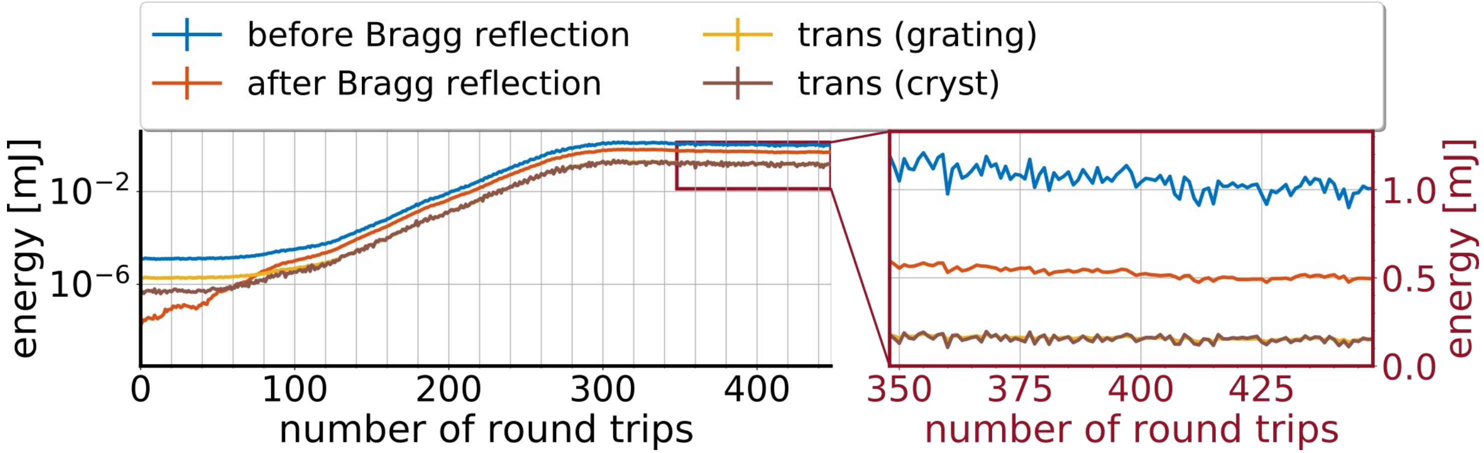
Including Thermal Response/ Introducing additional losses/outcoupling

- Adding 15% of additional losses before downstream mirror (grating scheme)
  - Matching pulse energy in saturation to 1mJ
- Stable operation could be achieved
  - Reduced pulse energy



Simulation results	
Transmitted (grating)	
Sat. pulse energy	0.16(1) mJ
Spectral Q density	~30 µJ/THz
Brilliance	1.9(2)*10^{33}
Transmitted (cryst)	
Sat. pulse energy	0.15(2) mJ
Spectral Q density	~4 µJ/THz
Brilliance	1.7(4)*10^{33}
SASE	
Sat. pulse energy	~3 mJ
Spectral Q density	~0.5 µJ/THz
Brilliance	~5*10^{33}

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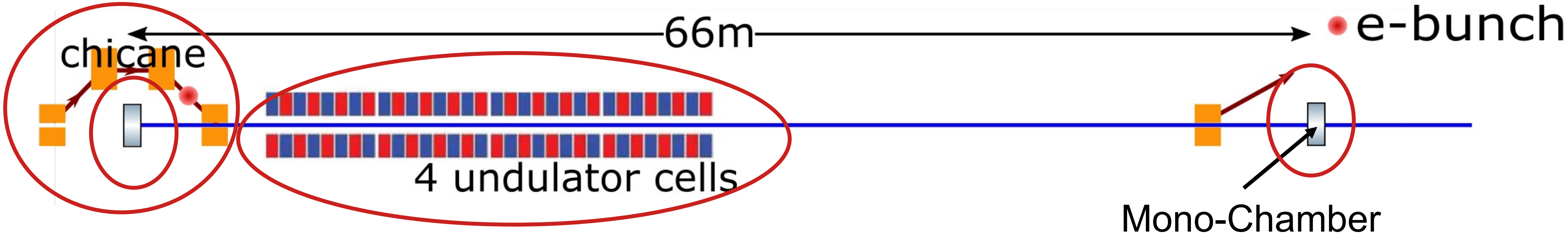
The Challenges of Alignment



- Undulators and chicane need dedicated alignment and optimization ←lot of experience from operations
- Monochromator alignment: Very challenging due to tight positional tolerances

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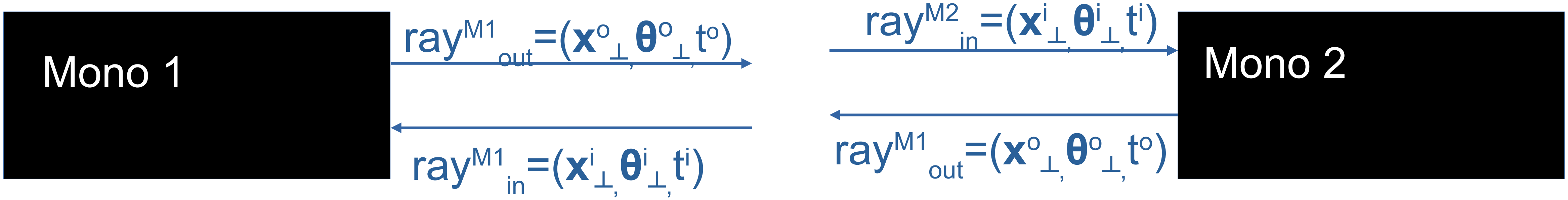
Monochromators: Relevant Degrees of Freedom



- Action of Mono 1:
  - Transverse shift: $\mathbf{x}^{o}_{\perp}=\mathbf{x}^{i}_{\perp}+\Delta\mathbf{x}_{\perp}$
  - Tilt: $\boldsymbol{\theta}^{o}_{\perp}=\boldsymbol{\theta}^{i}_{\perp}+\Delta\boldsymbol{\theta}_{\perp}$
  - Time shift: $t^{o}_{\perp}=t^{i}+\Delta t$

- Action of Mono 2:
  - Transverse shift: $\mathbf{x}^{o}_{\perp}=\mathbf{x}^{i}_{\perp}+\Delta\mathbf{x}_{\perp}$
  - Tilt: $\boldsymbol{\theta}^{o}_{\perp}=\boldsymbol{\theta}^{i}_{\perp}+\Delta\boldsymbol{\theta}_{\perp}$
  - Time shift: $t^{o}_{\perp}=t^{i}+\Delta t$

- Action of Mono 1 + Mono 2:
  - $\mathrm{ray}^{M1}_{out} = \mathrm{ray}^{M2}_{in} + (\Delta\mathbf{x}_{\perp}, \Delta\boldsymbol{\theta}_{\perp}, \Delta t)$

$\Delta\mathbf{x}_{\perp}$ [μm]	$\Delta\boldsymbol{\theta}_{\perp}$ [nrad]	Δz [μm]
10	200	10

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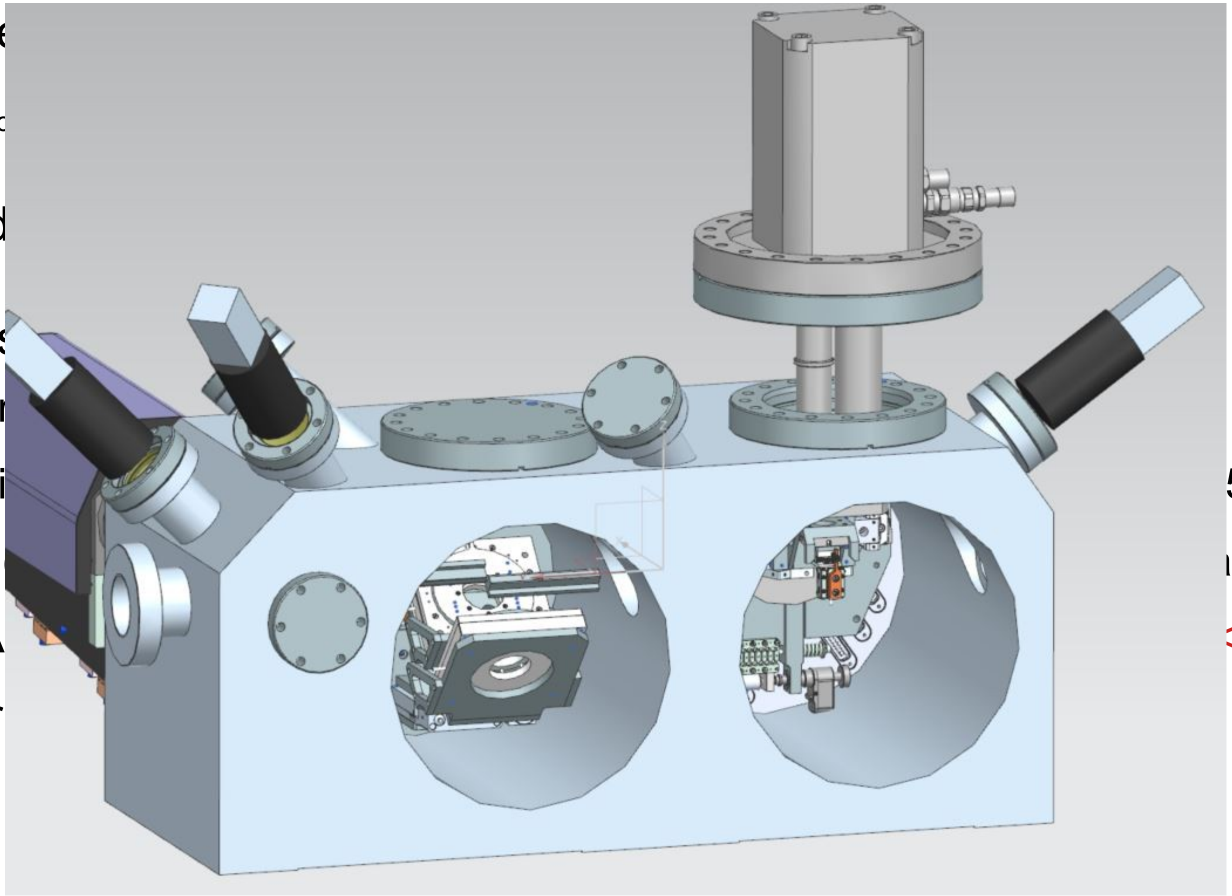
Individual Monochromators’ Errors

- Tolerance differe
  $(\Delta P,\Delta R)_{\mathrm{single}} =(P_{c}$
- Distance error d
- Alignment errors
  - Distance error
  - Common devi 5µm: $\Delta R, \Delta P < 10\mu\mathrm{rad}$
  - Yaw error $\Delta\alpha$ d: $\Delta\alpha < 2.5\mathrm{mrad}$
  - Diadic error Δ $<$ 1mrad
  - Positioning er



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How to achieve tolerances?

1. Rough pre-alignment (in and out of tunnel):
   - Tolerance difference pitch P and roll R between crystals and Kbs: $(\Delta P,\Delta R)_{single} = (P_c - P_{KB}, R_c - R_{KB}) \leq 100\,\mathrm{nrad}$
   - Distance error downstream and upstream Mono: $\Delta z \leq 10\,\mu m$: pre-alignment to $\Delta z \leq 0.5\,mm$
   - Alignment errors on Kbs:
     - Distance error $\Delta l \rightarrow (\Delta x,\Delta y)_{out} = 2*(\mathrm{Roll, Pitch})_C*\Delta l < 5\,\mu m$: $\Delta l < 1\,mm$
     - Common deviation Pitch, Roll from design $(\Delta R,\Delta P)$: $(\Delta x,\Delta y)_{out} = 2*(\Delta R,\Delta P)*l < 5\,\mu m$: $\Delta R,\Delta P < 10\,\mu rad$
     - Yaw error $\Delta\alpha$ ($@\alpha=-\pi/4$): $(\Delta R,\Delta P)[\Delta\alpha] \approx (-\sin(\theta_{in})\cdot\Delta\alpha^2/\sqrt{2}, \sqrt{2}\cdot\sin(\theta_{in})\cdot\Delta\alpha) < 10\,\mu rad$: $\Delta\alpha < 2.5\,mrad$
     - Diadic error $\Delta\alpha_d$($@\alpha=-\pi/4$): $(\Delta R,\Delta P)[\Delta\alpha_d] = (0, 2\cdot\sqrt{2}\cdot\sin(\theta_{in})\cdot\Delta\alpha_d) < 10\,\mu rad$: $\Delta\alpha_d < 1\,mrad$
     - Positioning error $(\Delta x,\Delta y)_{KB}$: $(\Delta x,\Delta y)_{out} \approx 2*(\Delta x,\Delta y)_{KB} < 5\,\mu m$: $\Delta x_{KB},\Delta y_{KB} < 2\,\mu m$

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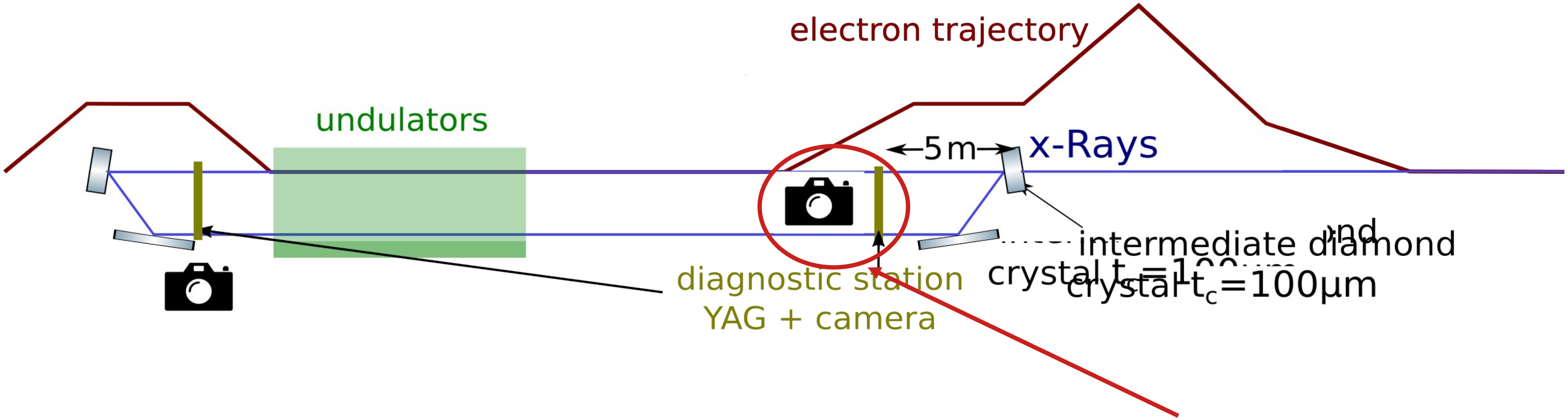
How to achieve tolerances?

1. Rough pre-alignment (in and out of tunnel):
2. In Tunnel Fine Alignment:



OTR-Chamber by MDI

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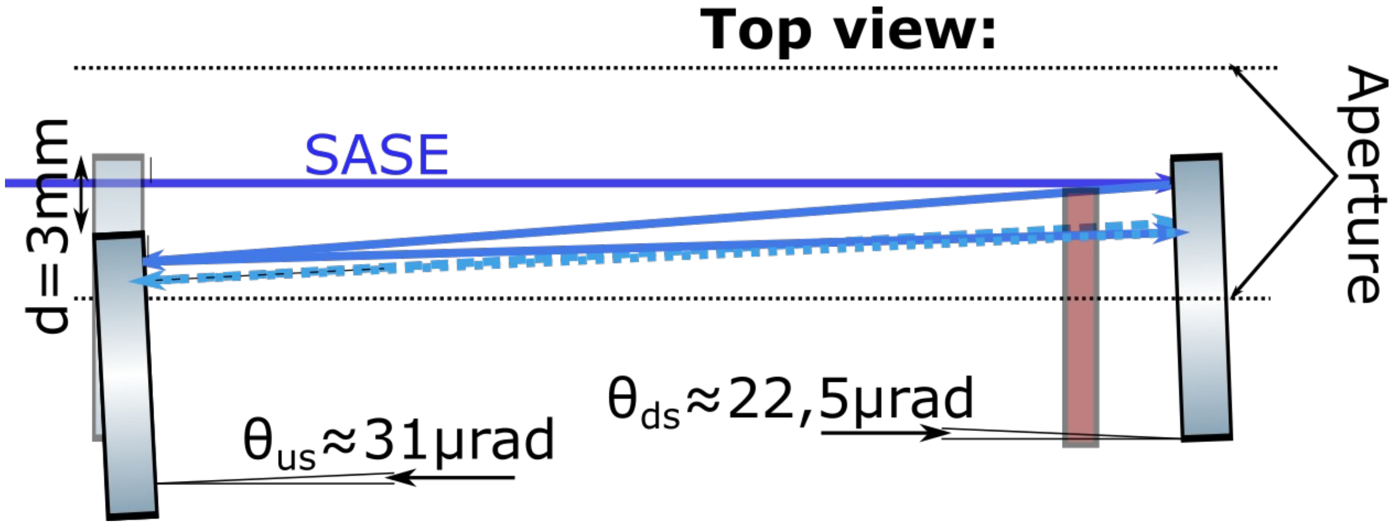
How to achieve tolerances?

1. Rough pre-alignment (in and out of tunnel):
2. In Tunnel Fine Alignment:
   i. Diamond Crystal Alignment
      - Tracking reflection *notches* using HIREX spectrometer ← $\Delta\theta_c \leq 1\,\mu\text{rad}$
      - Tracking beamspot after reflection of SASE beam using intra-cavity diagnostics ← **$\Delta\theta_c \leq 100\,\text{nrad}$**



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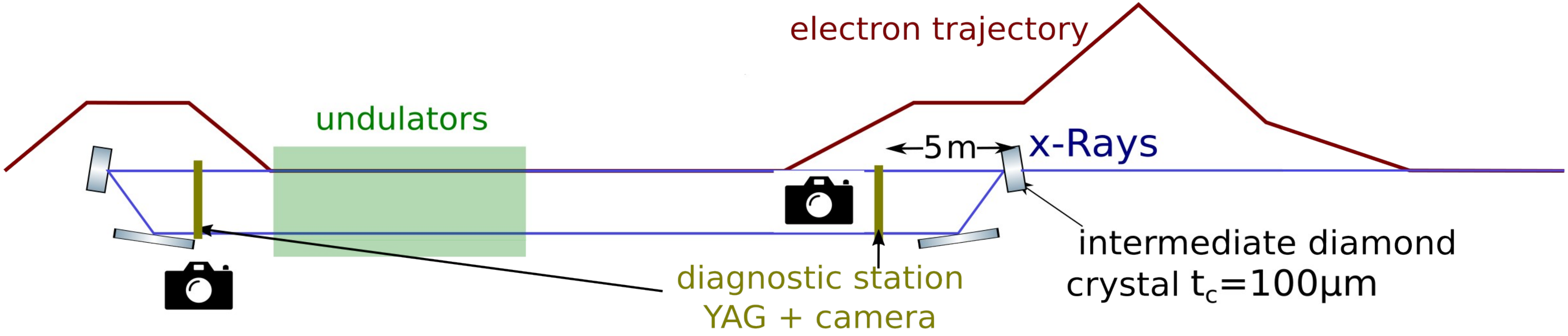
How to achieve tolerances?

1. Rough pre-alignment (in and out of tunnel):
2. In Tunnel Fine Alignment:
   1. Diamond Crystal Alignment ($\Delta\theta_c \leq 100\,\text{nrad}$)
   2. KB mirrors alignment tracking beamspot of inter-cavity radiation



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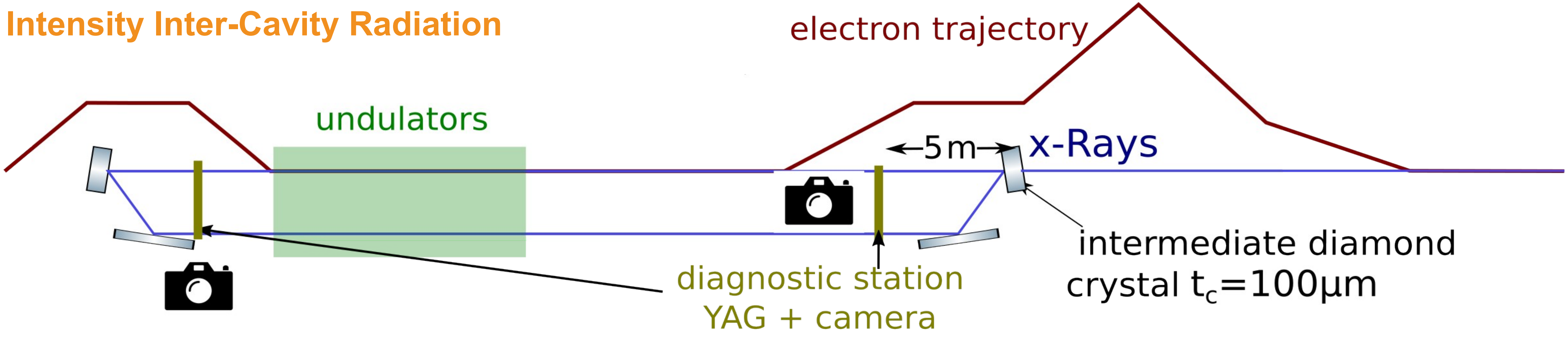
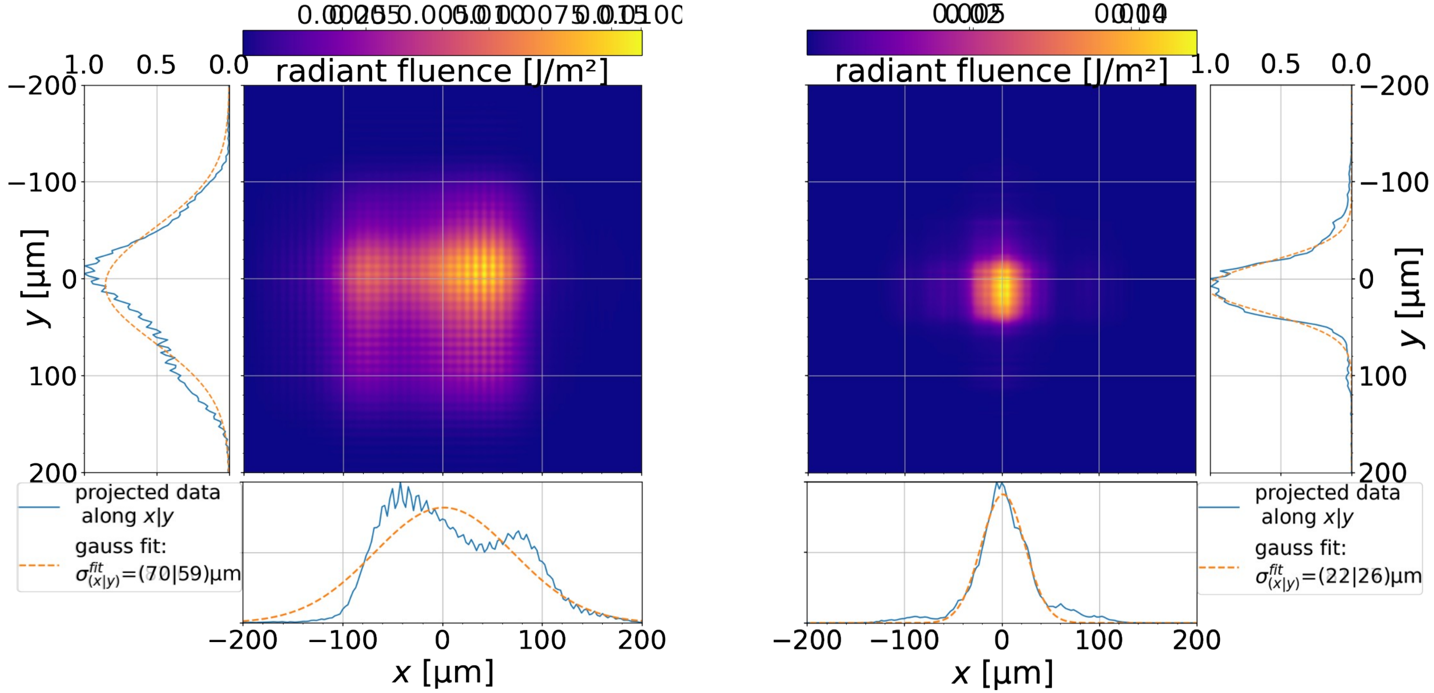
Low Intensity Inter-Cavity Radiation





- Low fluences!
  - By averaging: Enough SNR
  - BUT!: What is the optical background?
- Test beforehand: Installation of OTR chamber in winter shutdown 2022/2023

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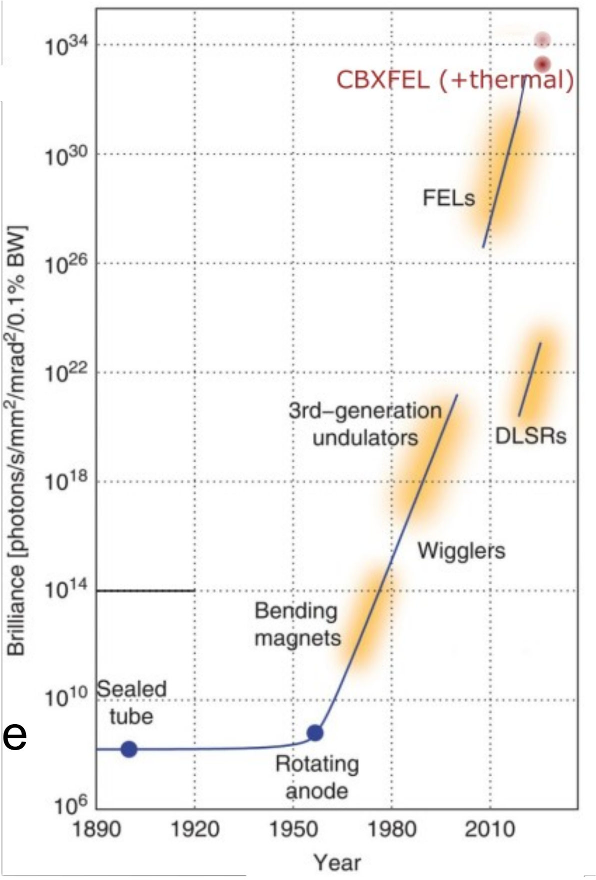
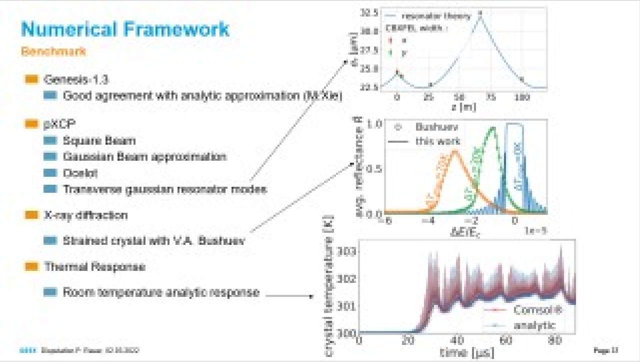
Summary

- CBXFEL promises outstanding radiation characteristics
  - Orders of magnitude higher peak spectral flux than SASE
  - High shot to shot stability
- European XFEL ideal facility for realization of an CBXFEL
- R&D project for implementing a proof of principle CBXFEL demonstrator
  - Simple setup with feasible (but demanding!) tolerances
- Experiment may deliver intense pulses with very high spectral flux
- Unstable operation/reduced pulse quality if incorporating crystals’ thermal response
- Demanding alignment based on individual component strategy
  - Lot of components to align with limited number of diagnostics
  - Low intensities



THANK YOU!

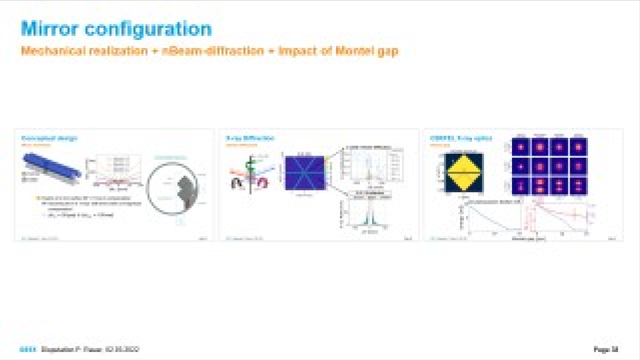
BACKUP



Numerical Framework

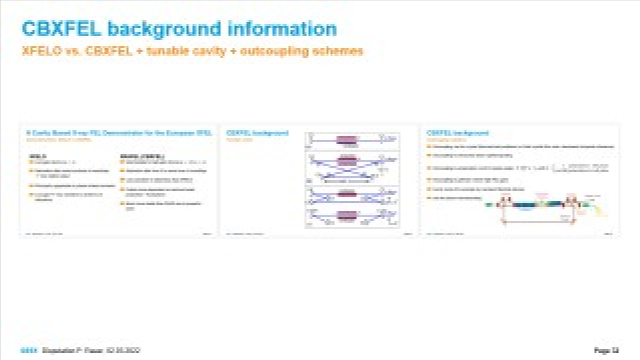
Benchmark

- Genesis-1.3
  - Good agreement with analytic approximation (M.Xie)
- pXCP
  - Square Beam
  - Gaussian Beam approximation
  - Ocelot
  - Transverse gaussian resonator modes
- X-ray diffraction
  - Strained crystal with V.A. Bushuev
- Thermal Response
  - Room temperature analytic response



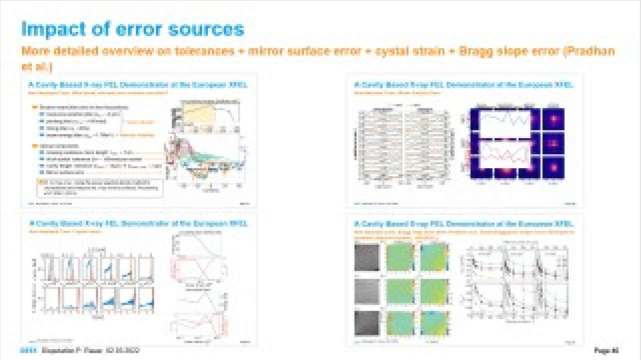
Mirror configuration

Mechanical realization + nBeam-diffraction + Impact of Montel gap



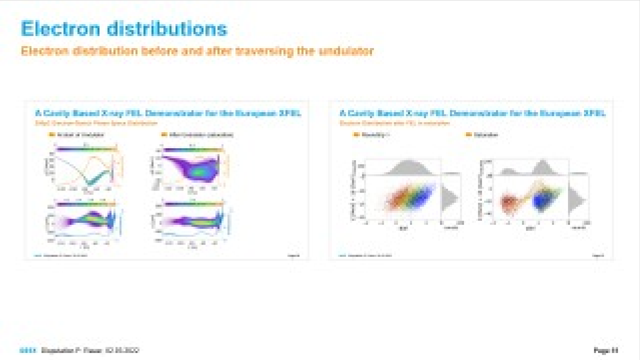
CBXFEL background information

XFELO vs. CBXFEL + tunable cavity + outcoupling schemes



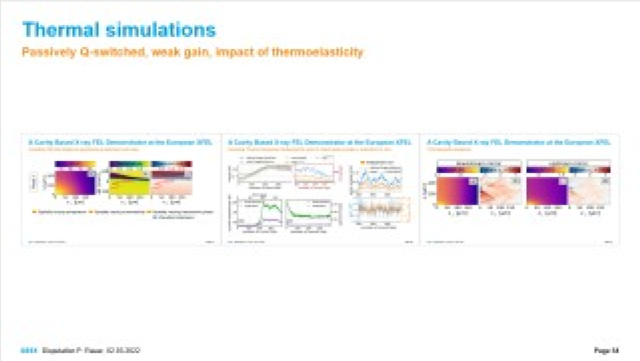
Impact of error sources

More detailed overview on tolerances + mirror surface error + cystal strain + Bragg slope error (Pradhan et al.)



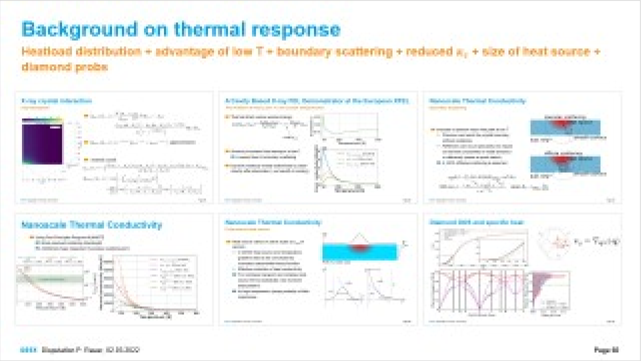
Electron distributions

Electron distribution before and after traversing the undulator



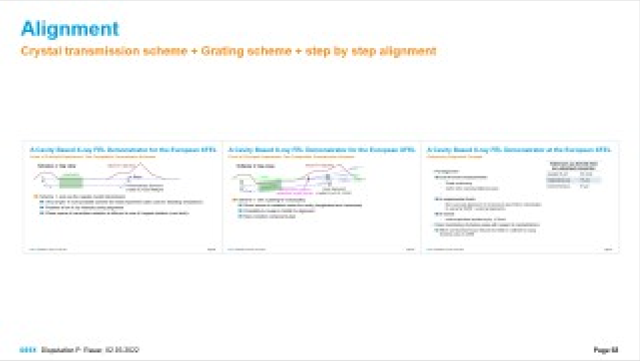
Thermal simulations

Passively Q-switched, weak gain, impact of thermoelasticity



Background on thermal response

Heatload distribution + advantage of low T + boundary scattering + reduced κ_l + size of heat source + diamond probe

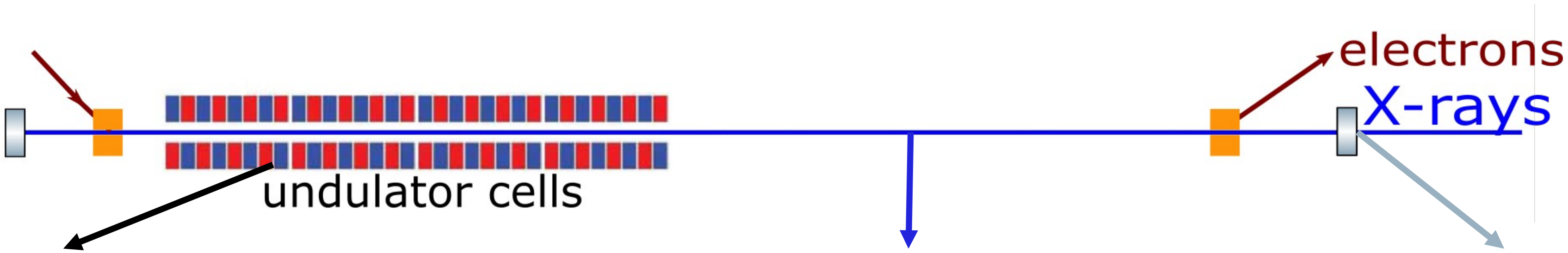


Alignment

Crystal transmission scheme + Grating scheme + step by step alignment

A Cavity Based X-ray FEL Demonstrator for the European XFEL

Start-2-End Modeling of a CBXFEL: Three Fully Coupled Submodules



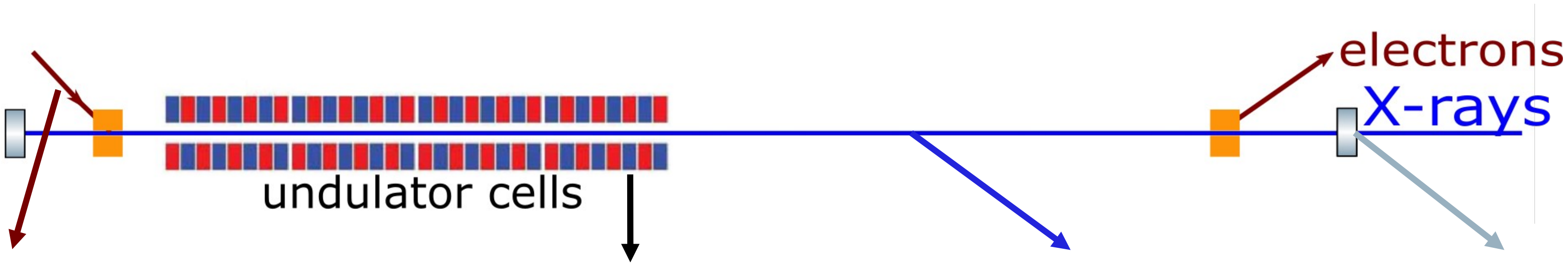
🟧 **FEL Process**

🟧 **X-ray Propagation**

🟧 **X-ray Crystal Interaction**

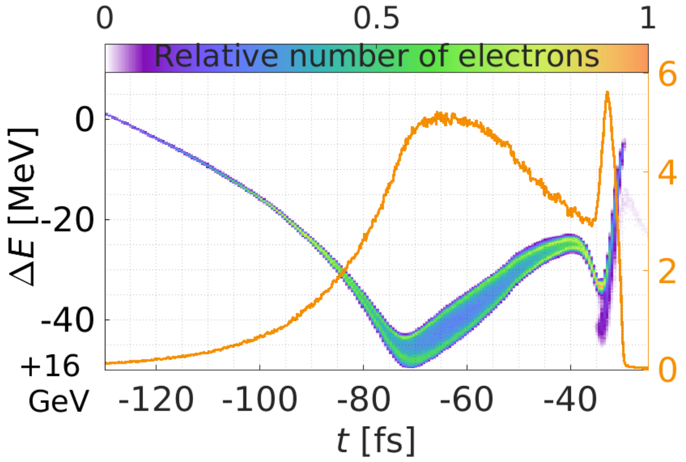
A Cavity Based X-ray FEL Demonstrator for the European XFEL

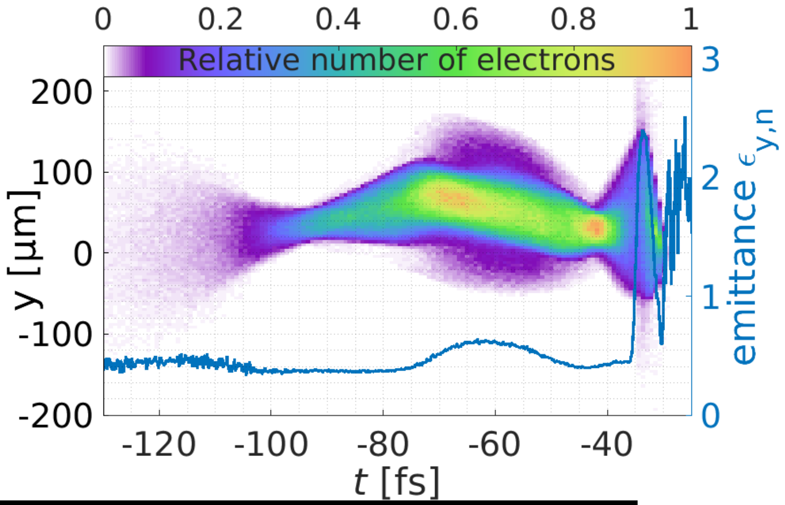
Start-2-End Modeling of a CBXFEL: Four Submodules



- **Electron Dynamics**
- **FEL Process**
- **X-ray Propagation**
- **X-ray Crystal Interaction**
  - Based on Start-2-End Simulations by I. Zagarodnov et al.

Simulation parameters	
Electron Energy	16 GeV
Bunch Charge	250 pC
FODO	32 m

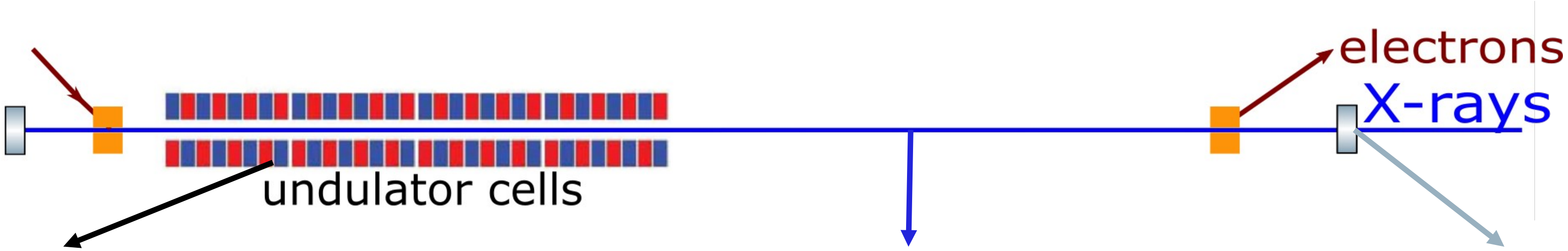




- Igor Zagorodnov et al., *Accelerator beam dynamics at the European X-ray Free Electron Laser*, PRAB (2019)

A Cavity Based X-ray FEL Demonstrator for the European XFEL

Start-2-End Modeling of a CBXFEL: Three Fully Coupled Submodules (+1)



FEL Process

- Using *Genesis-1.3* (V4)
  - ▶ Well known and benchmarked
  - ▶ Parallelized and fast
  - ▶ Many tunable parameters and adjustable errors

X-ray Propagation

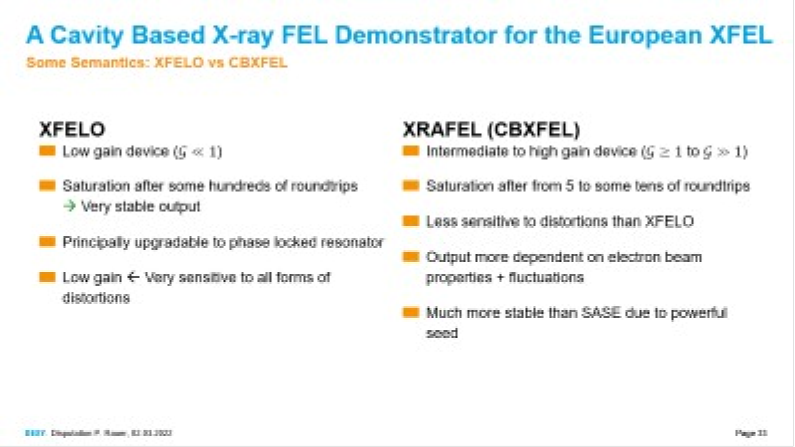
- Self-written *parallel X-ray Cavity Propagator* (pXCP)
  - ▶ Based on Fourier Optics
  - ▶ Very fast on (Maxwell) Cluster
  - ▶ Very versatile (adjustable optics and error sources)

X-ray Crystal Interaction

- X-ray reflection based on (two beam) dynamic diffraction
- Crystal thermal response using COMSOL Multiphysics®

CBXFEL background information

XFELO vs. CBXFEL + tunable cavity + outcoupling schemes



A Cavity Based X-ray FEL Demonstrator for the European XFEL

Some Semantics: XFELO vs CBXFEL

XFELO

- Low gain device ($\mathcal{G} \ll 1$)
- Saturation after some hundreds of roundtrips
  → Very stable output
- Principally upgradable to phase locked resonator
- Low gain ← Very sensitive to all forms of distortions

XRAFEL (CBXFEL)

- Intermediate to high gain device ($\mathcal{G} \geq 1$ to $\mathcal{G} \gg 1$)
- Saturation after from 5 to some tens of roundtrips
- Less sensitive to distortions than XFELO
- Output more dependent on electron beam properties + fluctuations
- Much more stable than SASE due to powerful seed

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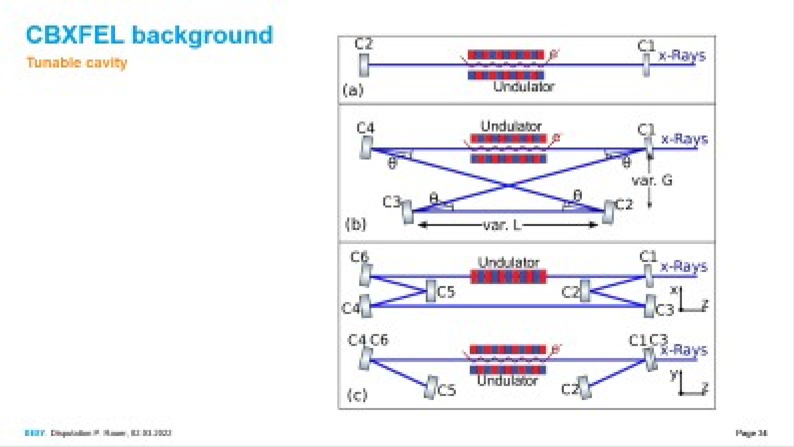

CBXFEL background

Tunable cavity

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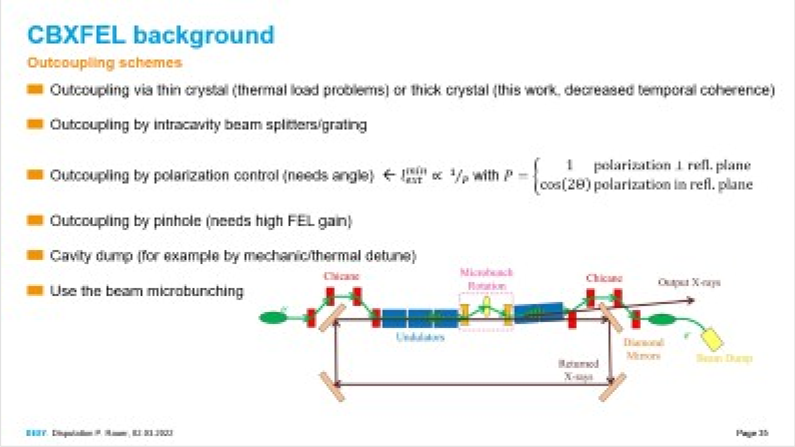

CBXFEL background

Outcoupling schemes

- Outcoupling via thin crystal (thermal load problems) or thick crystal (this work, decreased temporal coherence)
- Outcoupling by intracavity beam splitters/grating
- Outcoupling by polarization control (needs angle) ← $I_{ext}^{min} \propto {}^{1}/_{P}$ with $P = \begin{cases} 1 & \text{polarization} \perp \text{refl. plane} \\ \cos(2\theta) & \text{polarization in refl. plane} \end{cases}$
- Outcoupling by pinhole (needs high FEL gain)
- Cavity dump (for example by mechanic/thermal detune)
- Use the beam microbunching

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A Cavity Based X-ray FEL Demonstrator for the European XFEL

Some Semantics: XFELO vs CBXFEL

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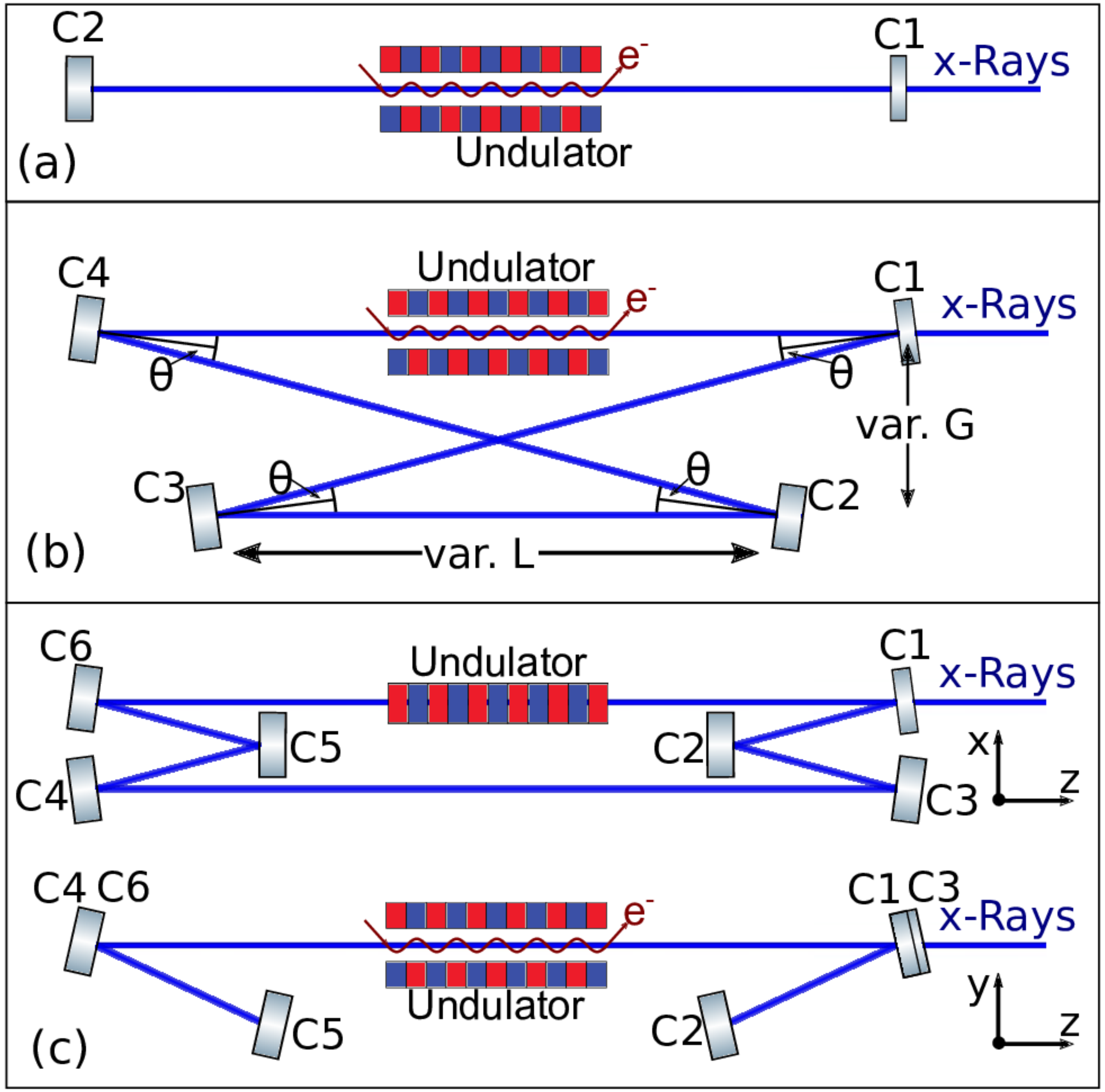
CBXFEL background

Tunable cavity



CBXFEL background

Outcoupling schemes

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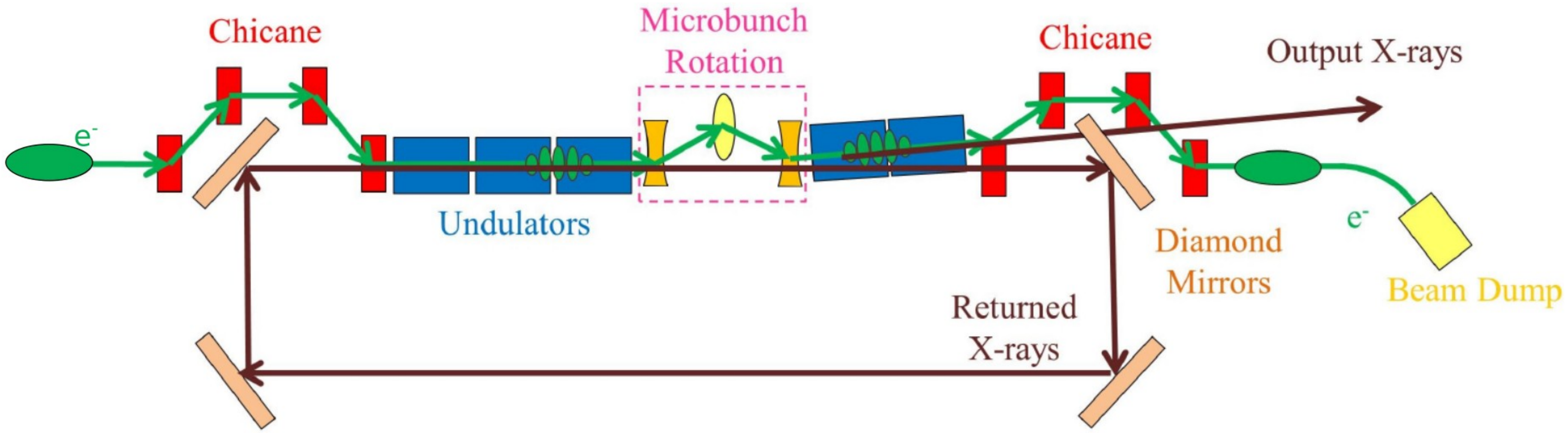
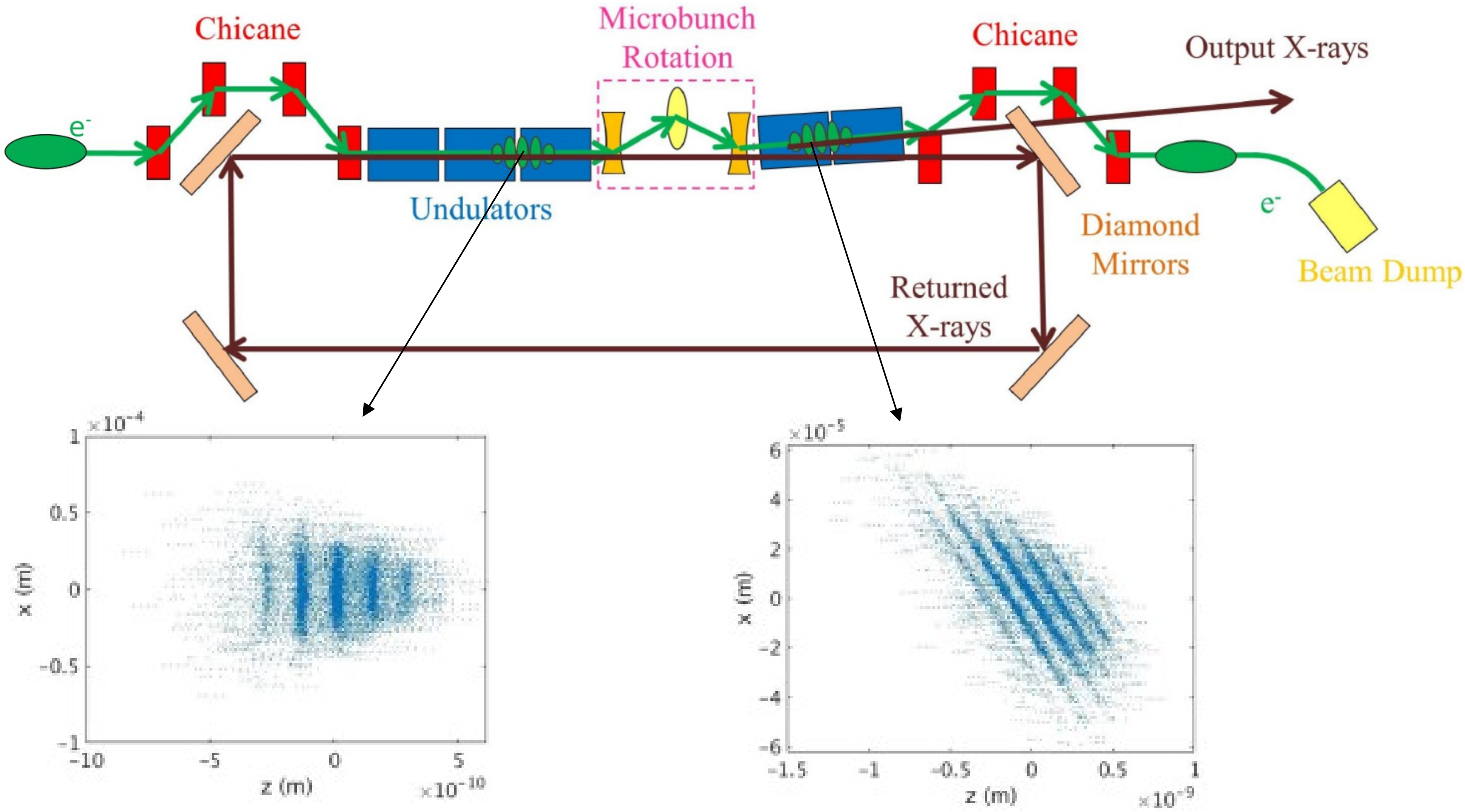
- Outcoupling by intracavity beam splitters/grating
- Outcoupling by polarization control (needs angle) ← with
- Outcoupling by pinhole (needs high FEL gain)
- Cavity dump (for example by mechanic/thermal detune)
- Use the beam microbunching



CBXFEL background

Outcoupling schemes: via Microbunching

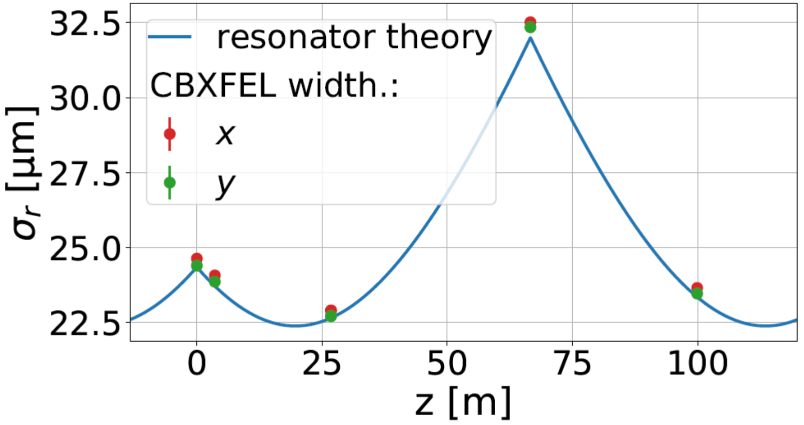
- Use the beam microbunching

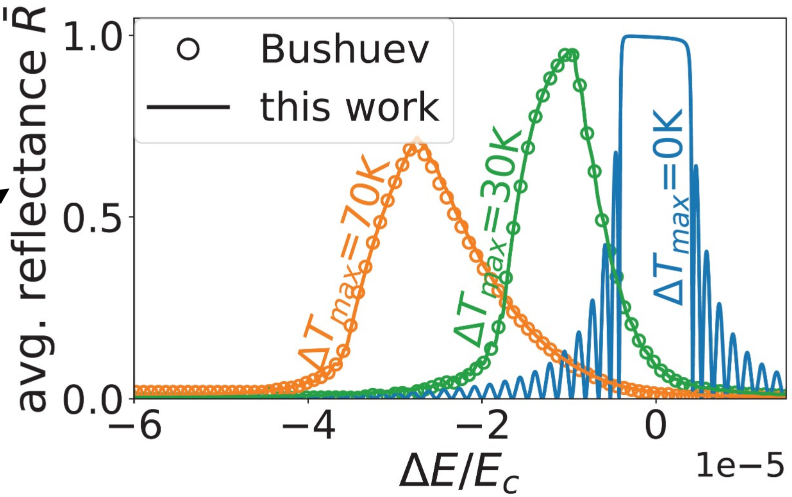


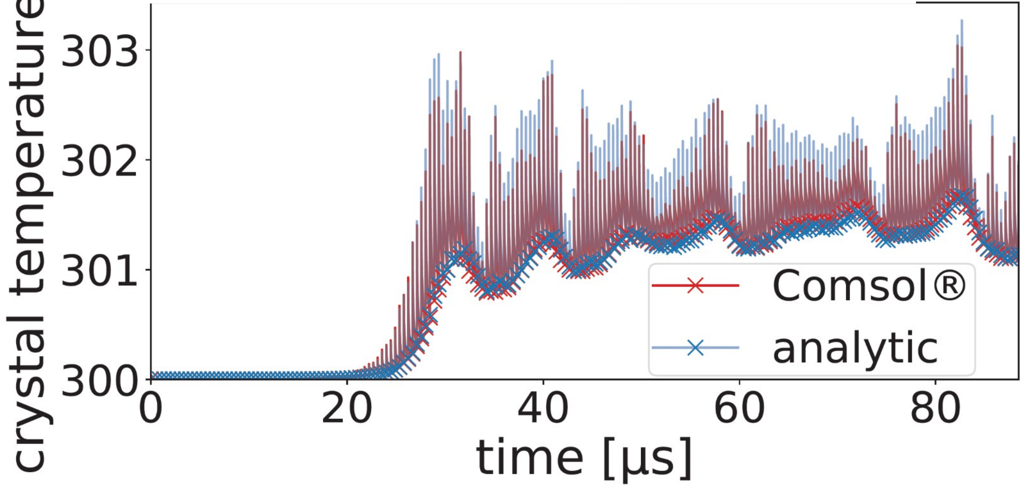
Numerical Framework

Benchmark

- Genesis-1.3
  - Good agreement with analytic approximation (M.Xie)
- pXCP
  - Square Beam
  - Gaussian Beam approximation
  - Ocelot
  - Transverse gaussian resonator modes
- X-ray diffraction
  - Strained crystal with V.A. Bushuev
- Thermal Response
  - Room temperature analytic response

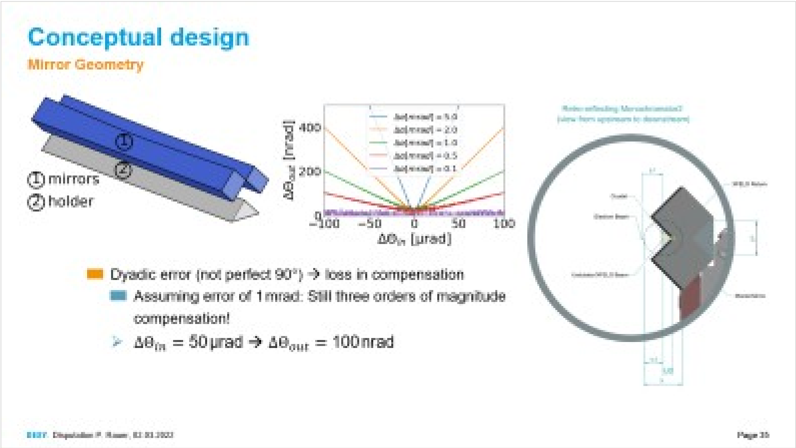






Mirror configuration

Mechanical realization + nBeam-diffraction + Impact of Montel gap



Conceptual design

Mirror Geometry

- Dyadic error (not perfect 90°) → loss in compensation
  - Assuming error of 1 mrad: Still three orders of magnitude compensation!
    - $\Delta\theta_{in}$ = 50 µrad → $\Delta\theta_{out}$ = 100 nrad

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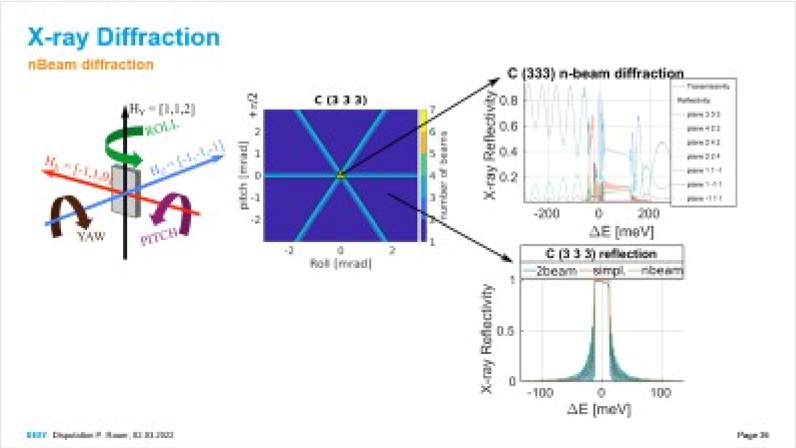

X-ray Diffraction

nBeam diffraction

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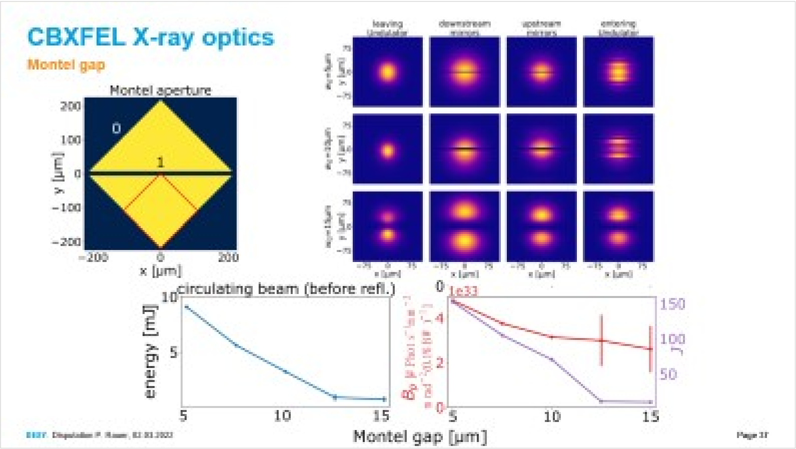

CBXFEL X-ray optics

Montel gap

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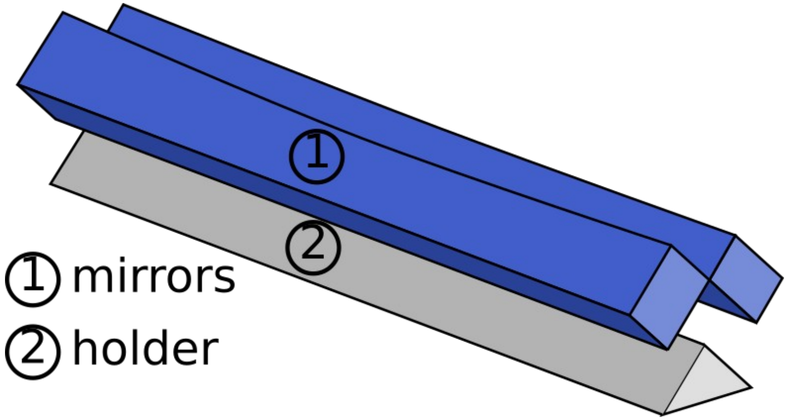
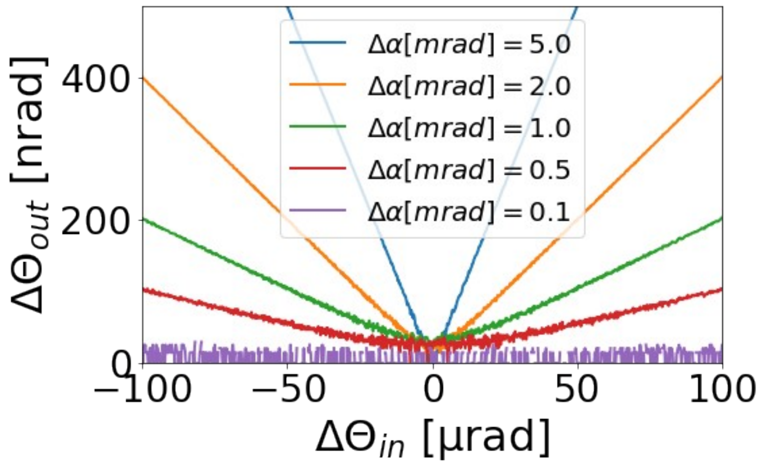
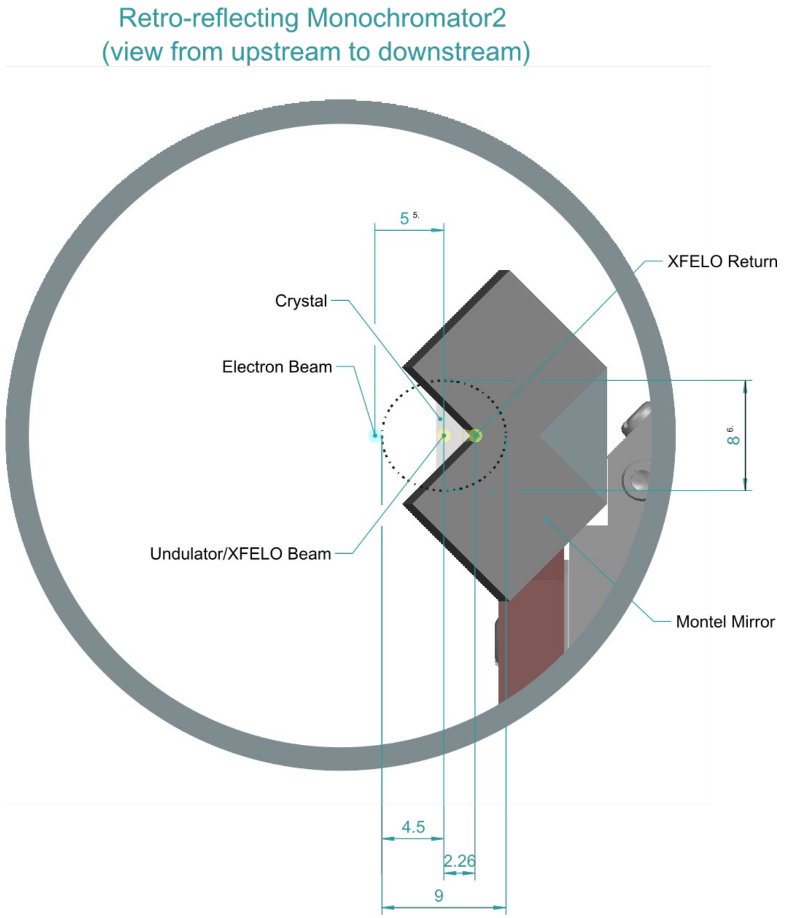
Conceptual design

Mirror Geometry



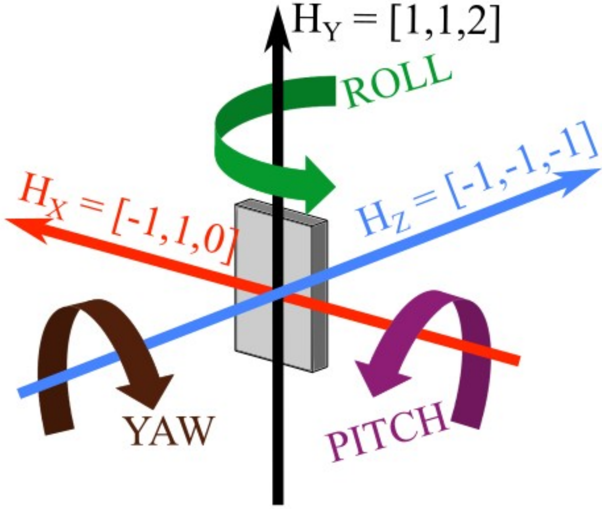


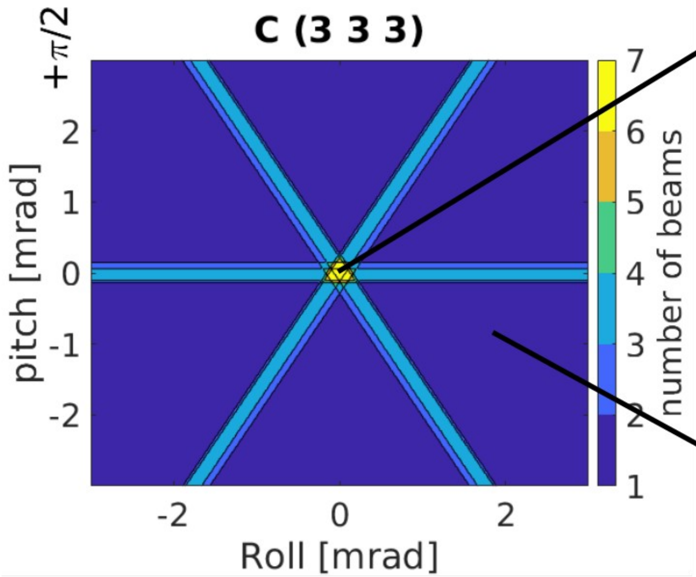

Retro-reflecting Monochromator2
(view from upstream to downstream)

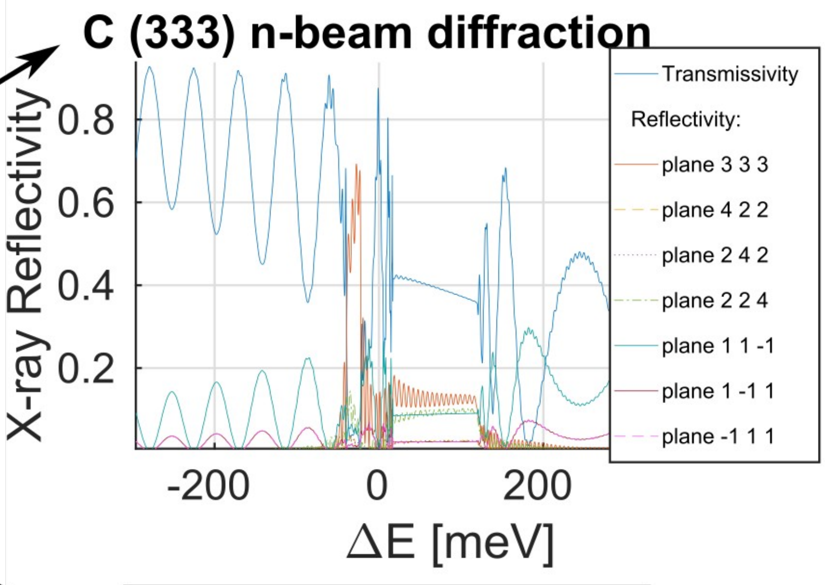
- Dyadic error (not perfect 90°) → loss in compensation
  - Assuming error of 1 mrad: Still three orders of magnitude compensation!
  - 50 µrad → 100 nrad

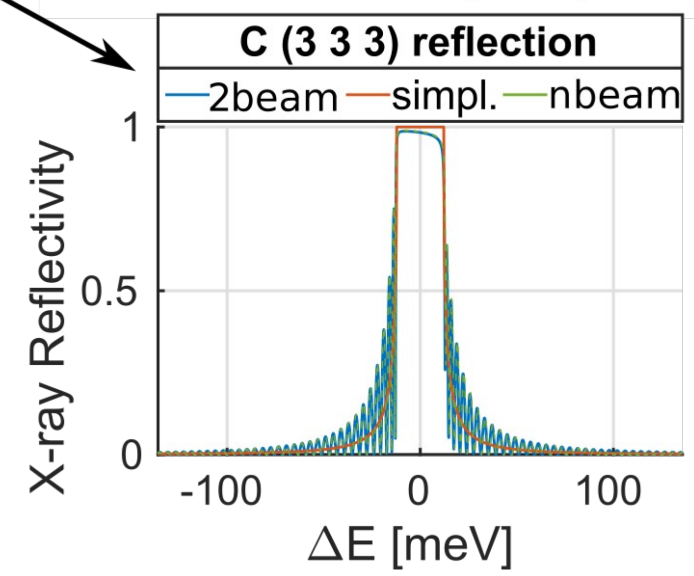
X-ray Diffraction

nBeam diffraction



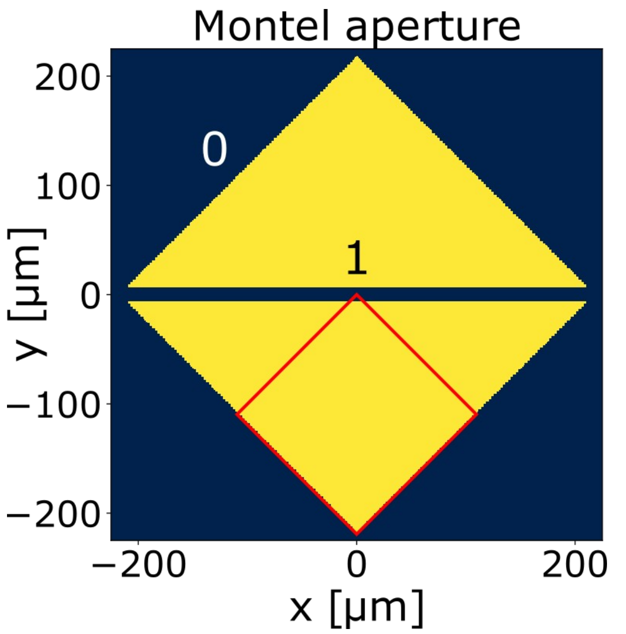


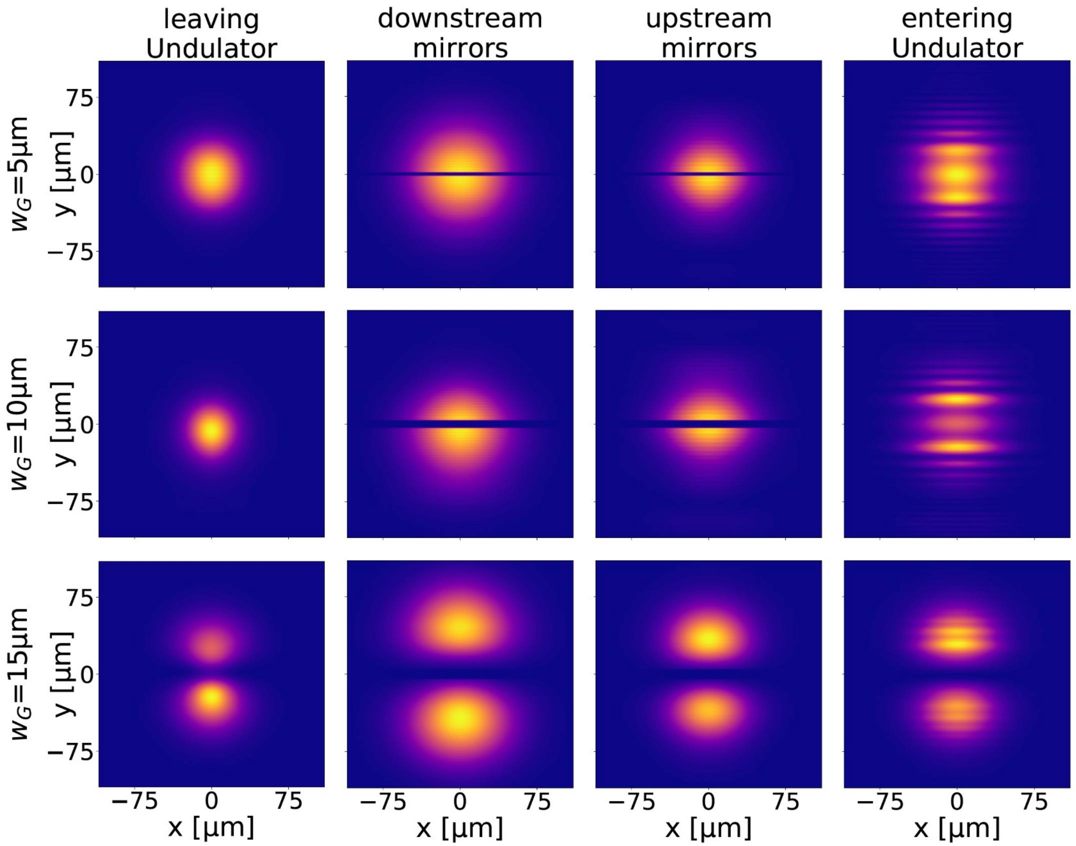


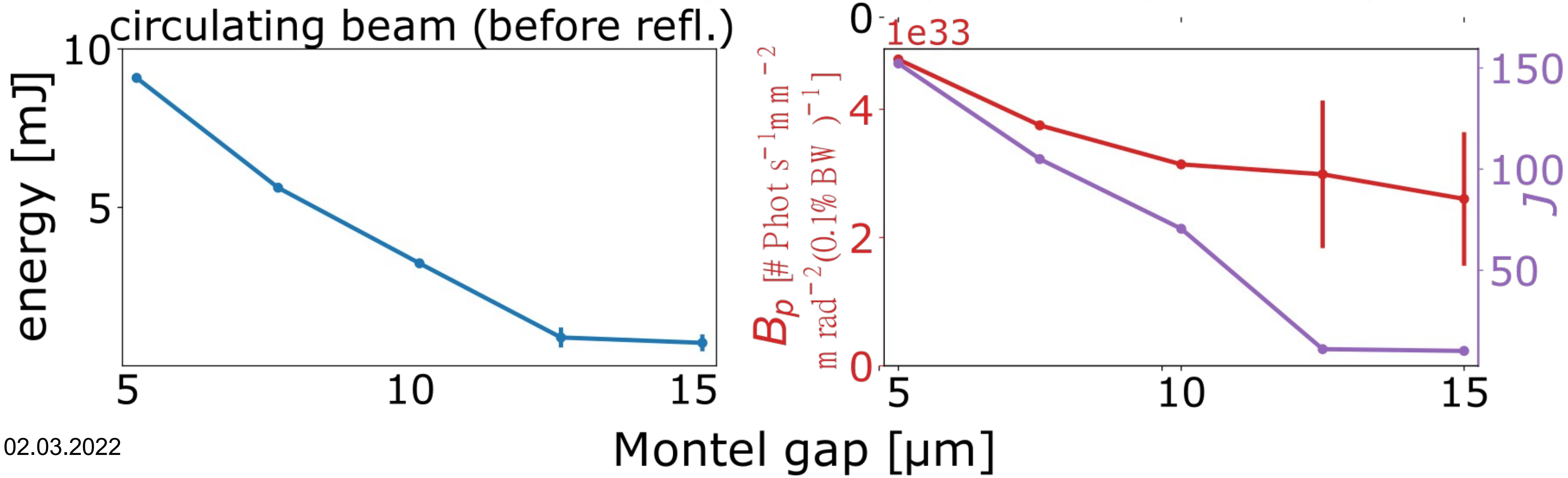


CBXFEL X-ray optics

Montel gap



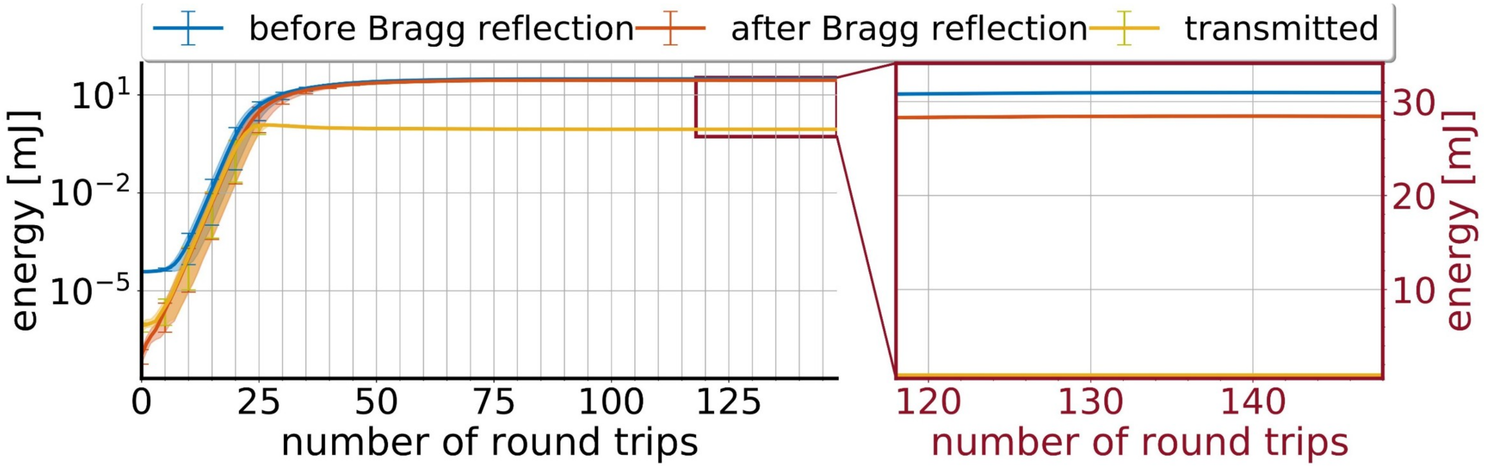


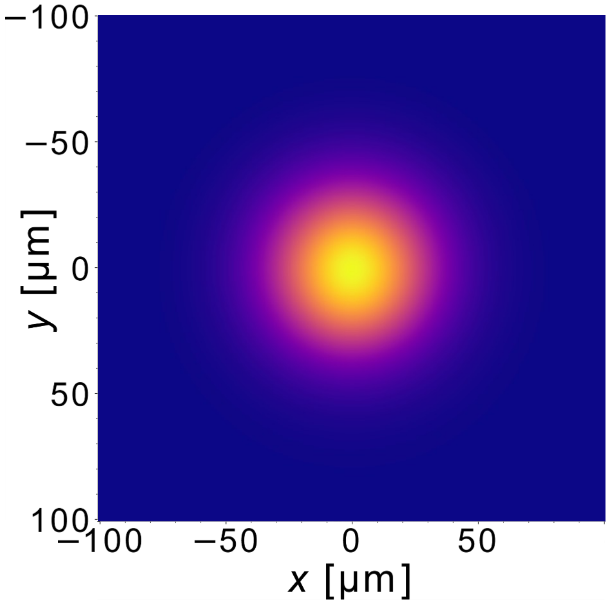


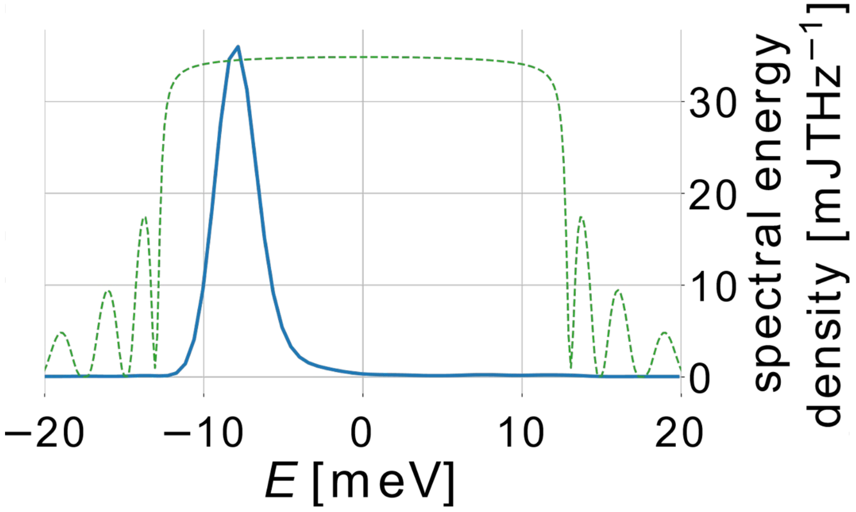
A Cavity Based X-ray FEL Demonstrator at the European XFEL

Idealized Case

Simulation results	
Before reflection	
Sat. pulse energy	31.5(1) mJ
spectral width	5.7(1) meV
rms duration	214(4) fs
-product (	1.85(7)
Brilliance	4.84(3)*10³⁶
Brilliance SASE	~5*10³³



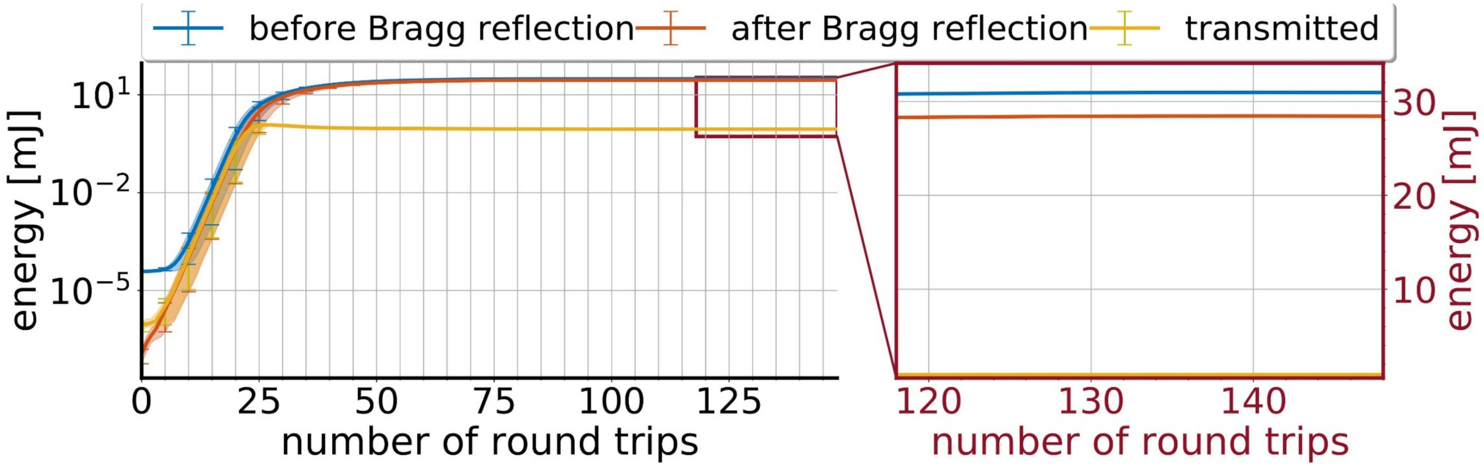


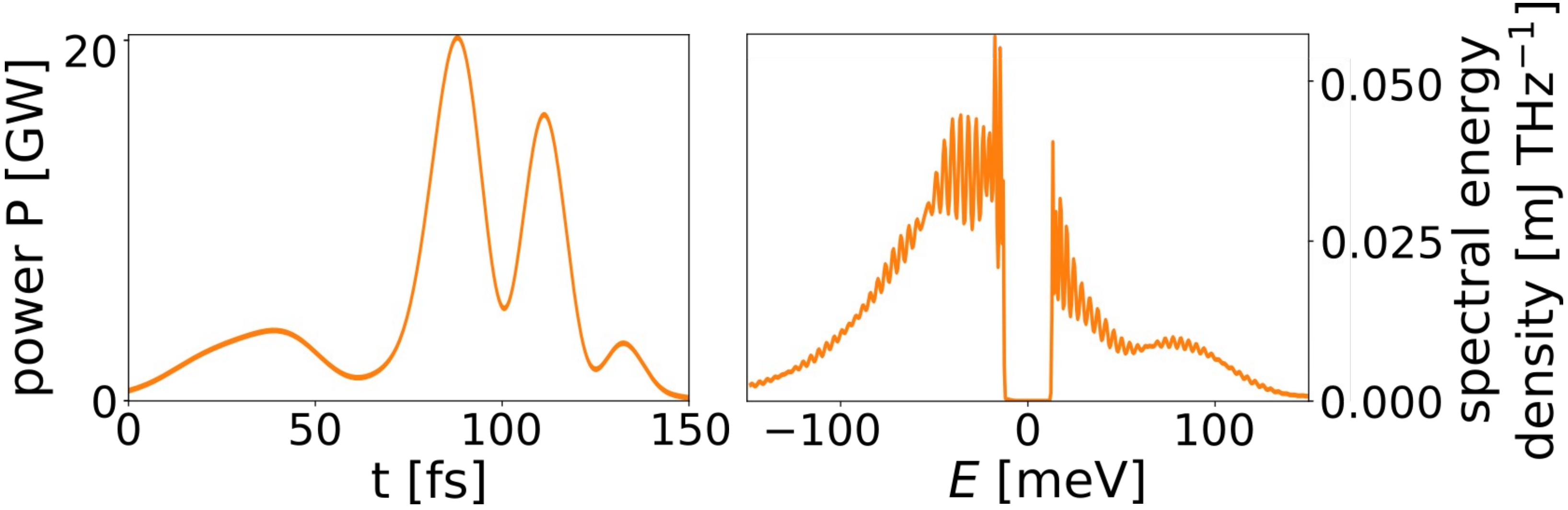


A Cavity Based X-ray FEL Demonstrator at the European XFEL

Idealized Case

Simulation results	
Before reflection	
Sat. pulse energy	31.5(1) mJ
spectral width	5.7(1) meV
rms duration	214(4) fs
-product (	1.85(7)
Brilliance	$4.84(3)*10^{36}$
Transmitted	
Sat. pulse energy	0.92(2) mJ
spectral width	60.3(4) meV
rms duration	123(4) fs
-product (	11.3(4)
Brilliance	$1.38(1)*10^{34}$
Brilliance SASE	$\sim5*10^{33}$



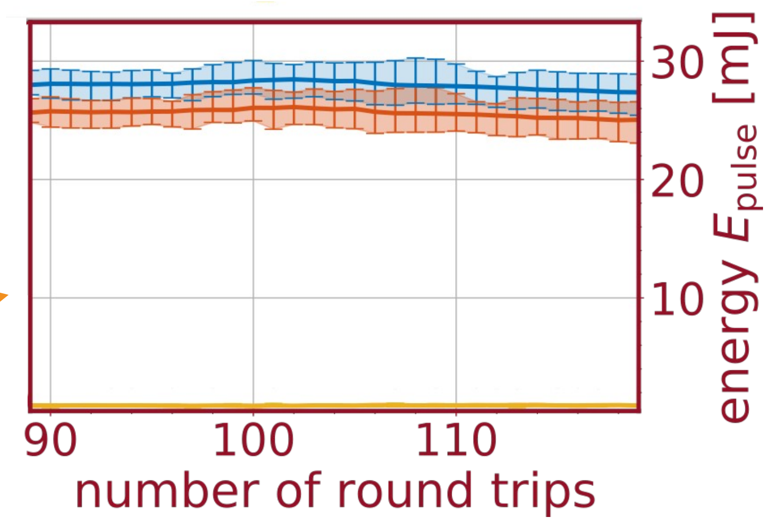


A Cavity Based X-ray FEL Demonstrator at the European XFEL

Non-Idealized Case: What (most relevant) error sources are there?

- Electron beam jitter (shot to shot fluctuations)
  - Transverse position jitter (3 µm)
  - Pointing jitter (100 nrad)
  - Timing jitter (20 fs)
  - Beam energy jitter (1.7 MeV)

quite robust!



A Cavity Based X-ray FEL Demonstrator at the European XFEL

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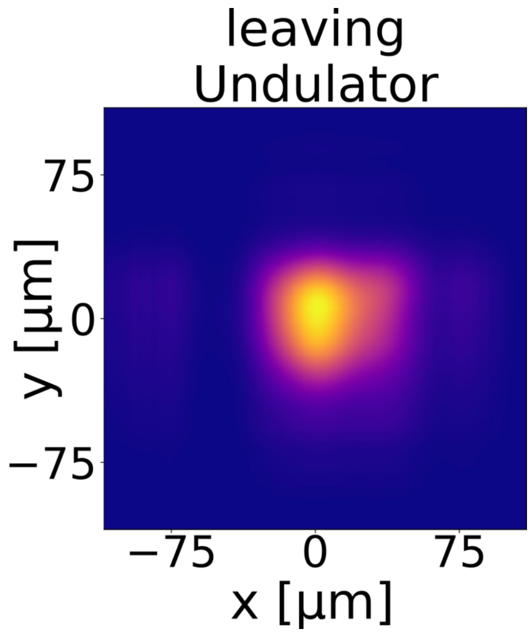
- Electron beam jitter (shot to shot fluctuations)
  - Transverse position jitter (3 µm)
  - Pointing jitter (100 nrad)
  - Timing jitter (20 fs)
  - Beam energy jitter (1.7 MeV) → **reduces stability**

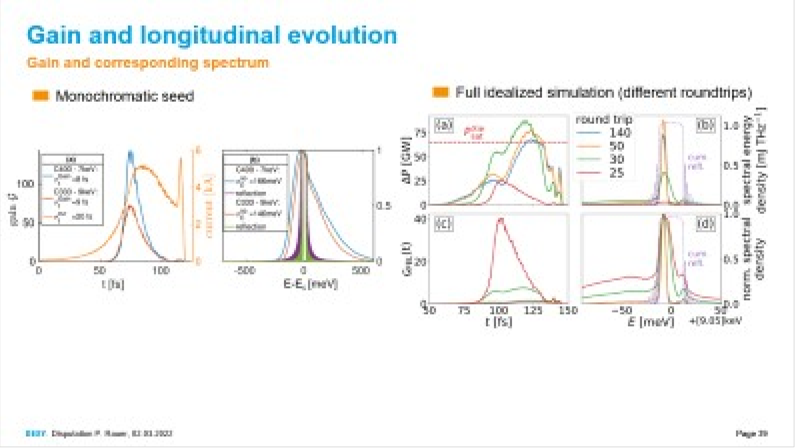
quite robust!

- Optical components
  - Grazing incidence mirror length: 14 cm
  - Tilt of crystal: tolerance 00 nrad per crystal
  - Cavity length: tolerance 0 µm → µm
  - Mirror surface error: 1.5 nm


leaving Undulator

Idealized Simulation

Gain evolution + oversaturation + improvement of transmitted pulse



Gain and longitudinal evolution

Gain and corresponding spectrum

- Monochromatic seed
- Full idealized simulation (different roundtrips)

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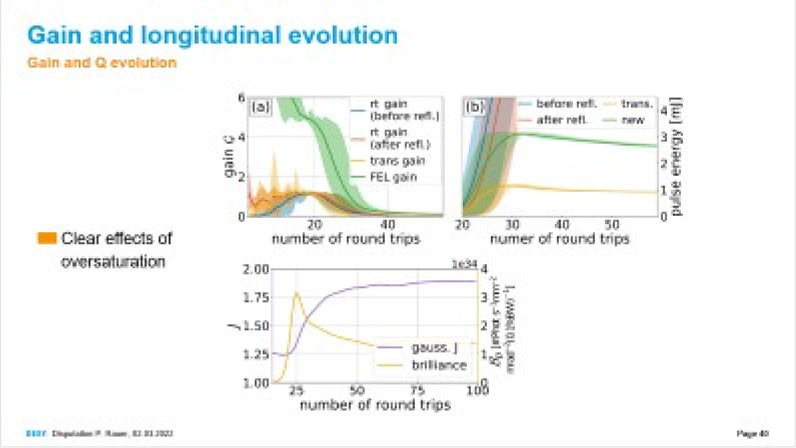

Gain and longitudinal evolution

Gain and Q evolution

- Clear effects of oversaturation

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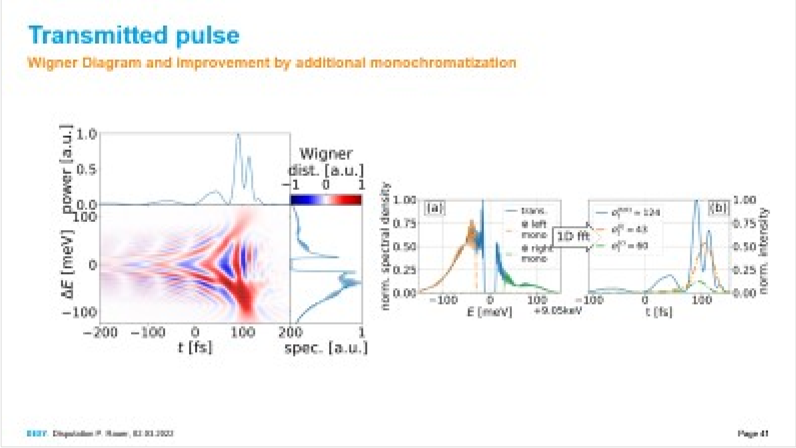

Transmitted pulse

Wigner Diagram and improvement by additional monochromatization

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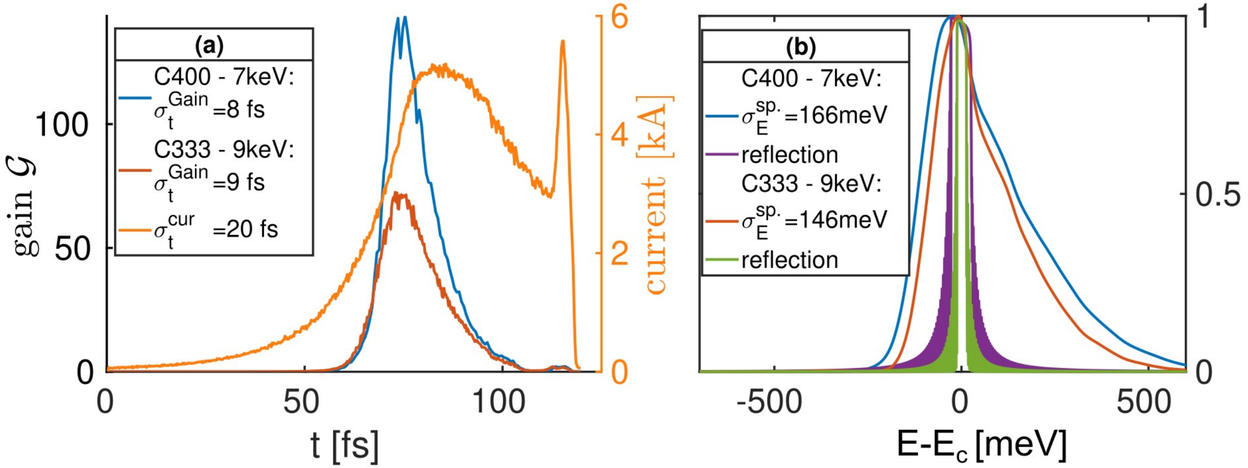
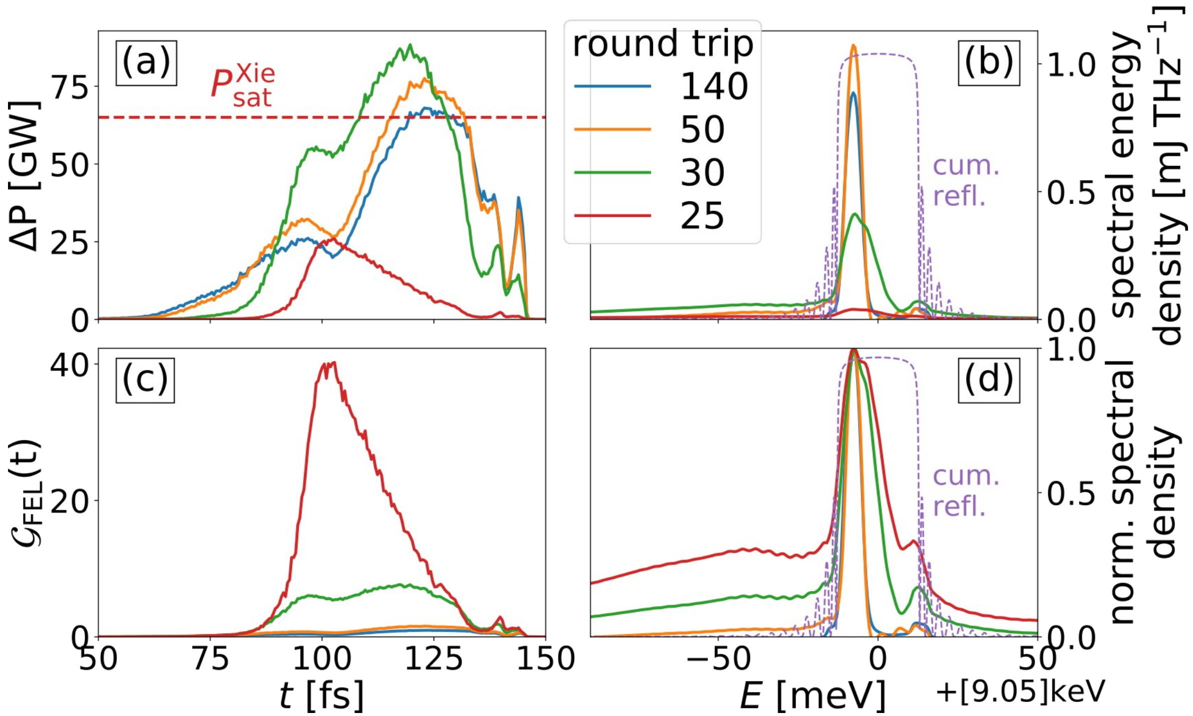
Gain and longitudinal evolution

Gain and corresponding spectrum

- Monochromatic seed

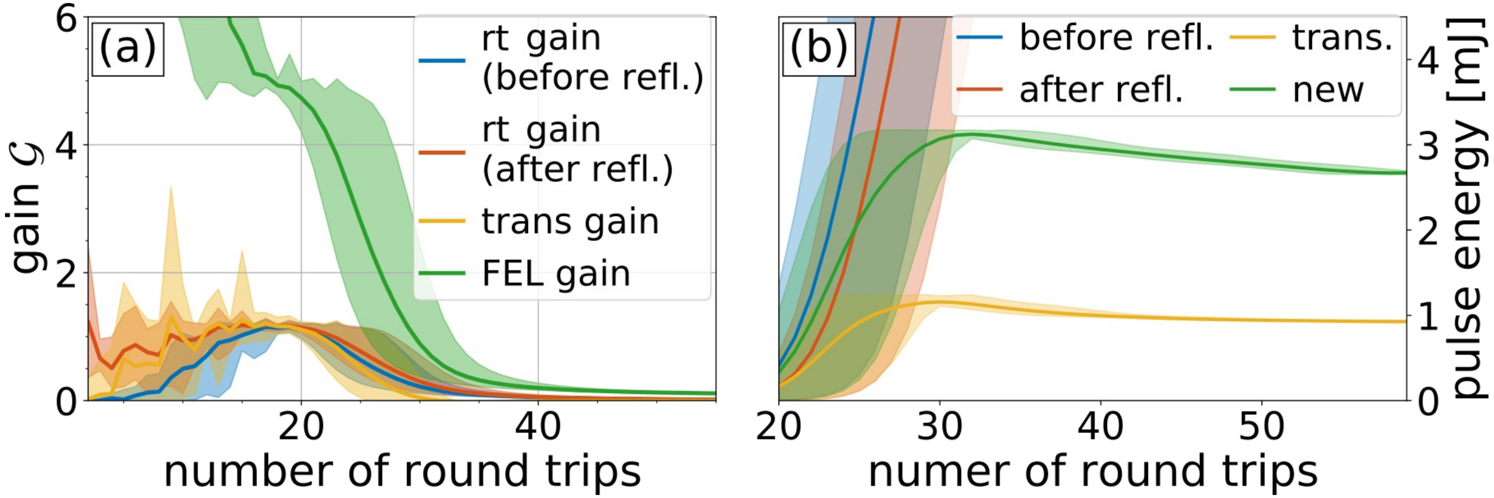


- Full idealized simulation (different roundtrips)

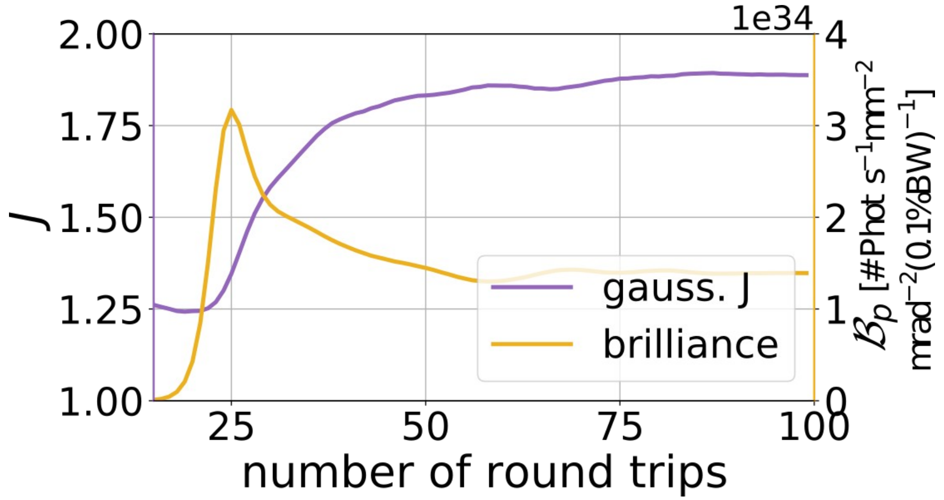


Gain and longitudinal evolution

Gain and Q evolution

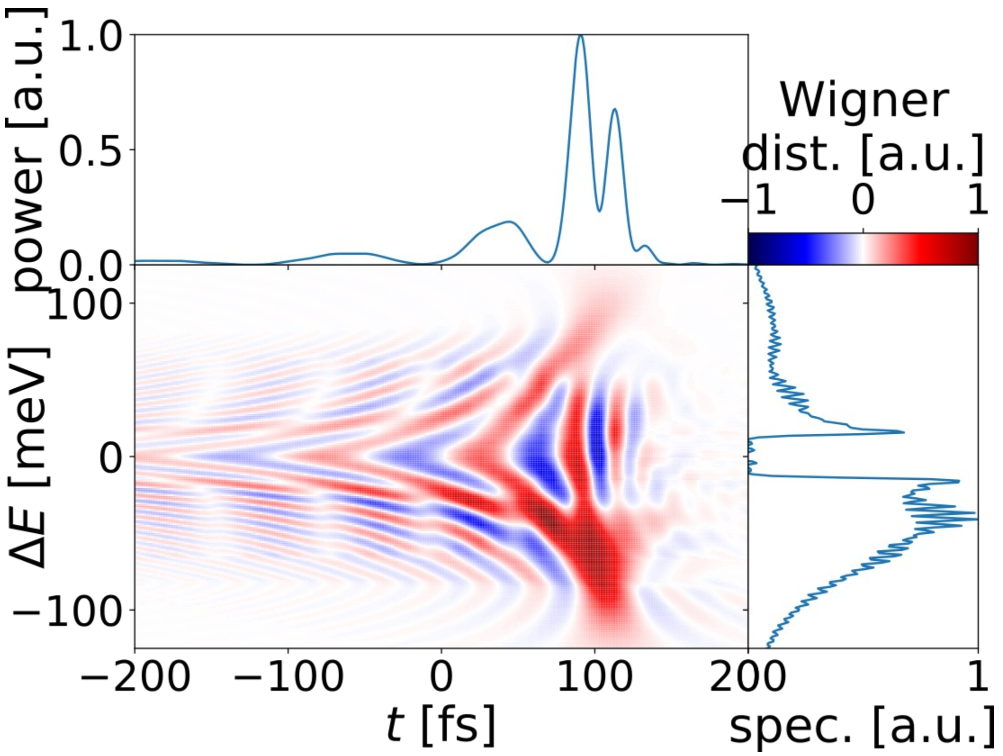


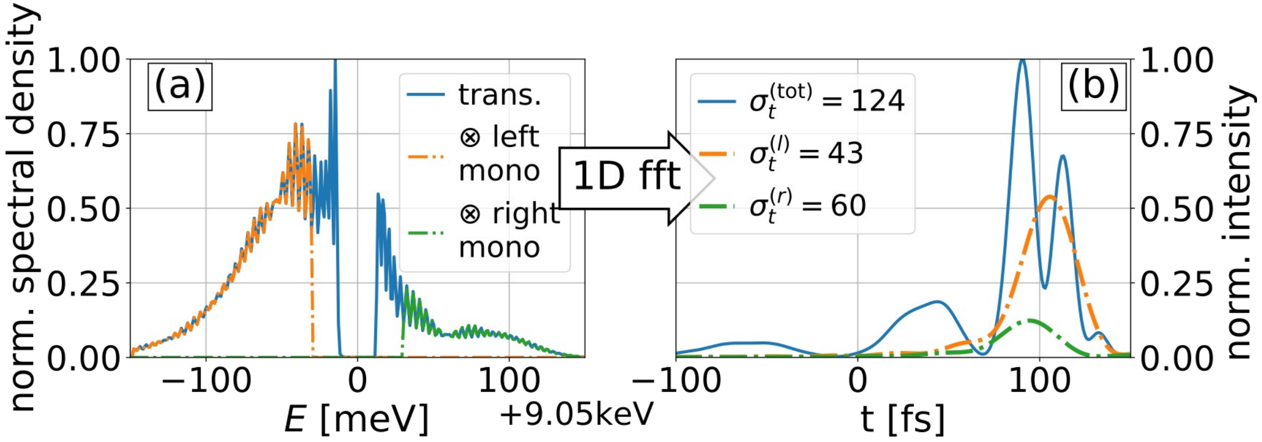
- Clear effects of oversaturation



Transmitted pulse

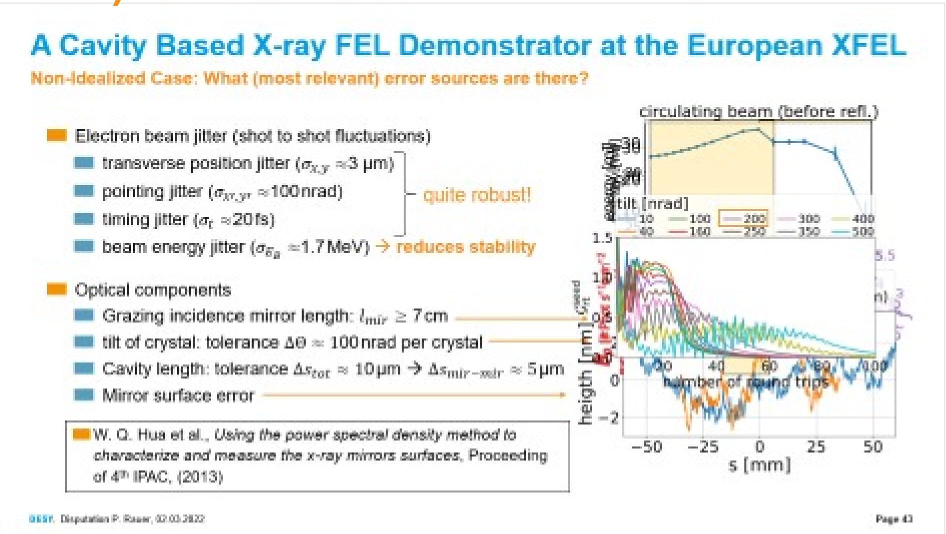
Wigner Diagram and improvement by additional monochromatization





Impact of error sources

More detailed overview on tolerances + mirror surface error + cystal strain + Bragg slope error (Pradhan et al.)



A Cavity Based X-ray FEL Demonstrator at the European XFEL

Non-Idealized Case: What (most relevant) error sources are there?

- Electron beam jitter (shot to shot fluctuations)
  - transverse position jitter ($\sigma_{x,y} \approx 3$ µm)
  - pointing jitter ($\sigma_{x',y'} \approx 100$ nrad)
  - timing jitter ($\sigma_t \approx 20$ fs)
  - beam energy jitter ($\sigma_{E_b} \approx 1.7$ MeV) → reduces stability

quite robust!

- Optical components
  - Grazing incidence mirror length: $l_{mir} \geq 7$ cm
  - tilt of crystal: tolerance $\Delta\Theta \approx 100$ nrad per crystal
  - Cavity length: tolerance $\Delta s_{tot} \approx 10$ µm → $\Delta s_{mir-mir} \approx 5$ µm
  - Mirror surface error

W. Q. Hua et al., *Using the power spectral density method to characterize and measure the x-ray mirrors surfaces*, Proceeding of 4th IPAC, (2013)

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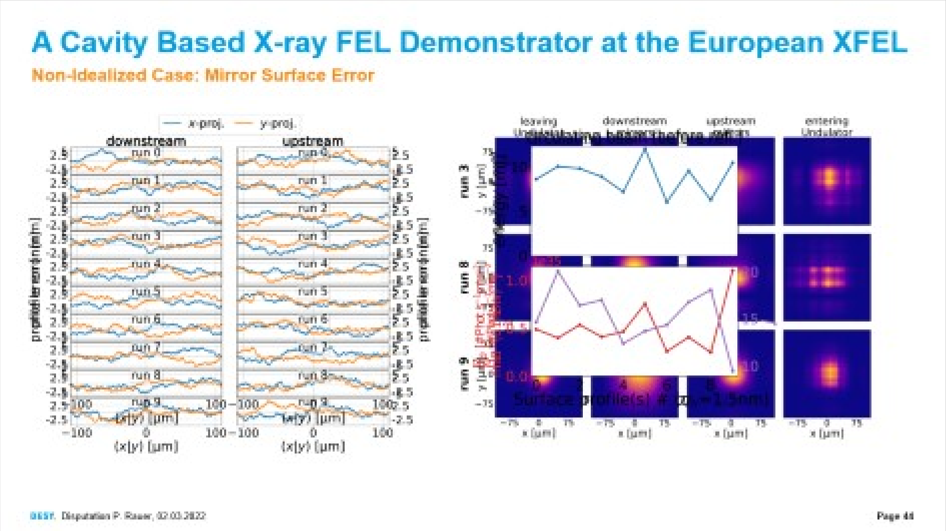

A Cavity Based X-ray FEL Demonstrator at the European XFEL

Non-Idealized Case: Mirror Surface Error

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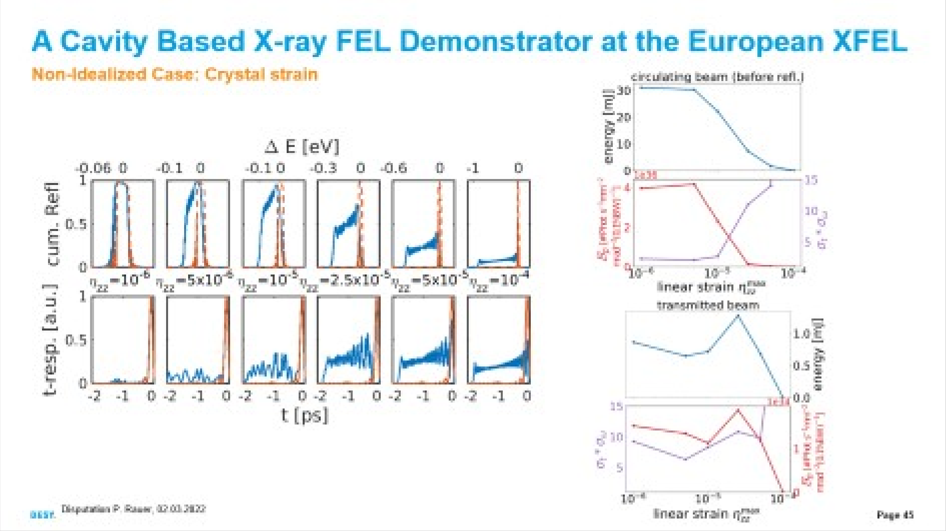

A Cavity Based X-ray FEL Demonstrator at the European XFEL

Non-Idealized Case: Crystal strain

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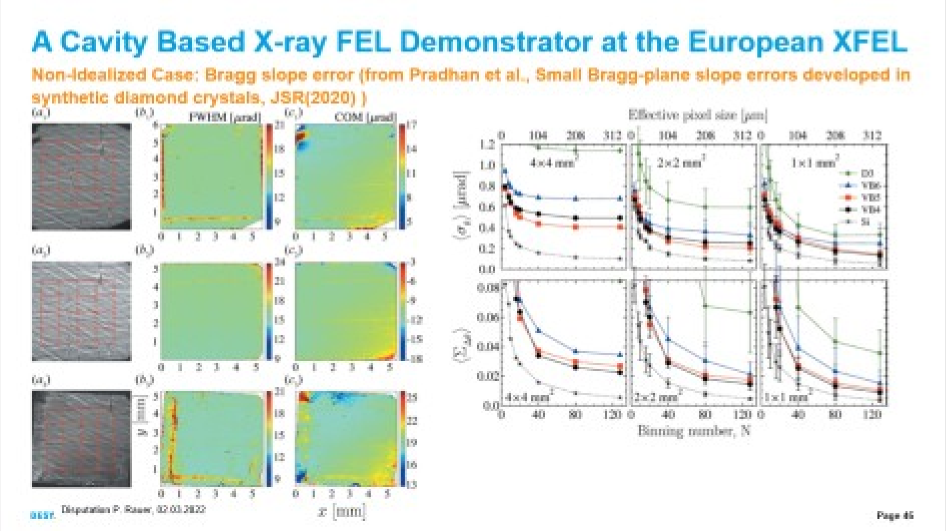

A Cavity Based X-ray FEL Demonstrator at the European XFEL

Non-Idealized Case: Bragg slope error (from Pradhan et al., Small Bragg-plane slope errors developed in synthetic diamond crystals, JSR(2020))

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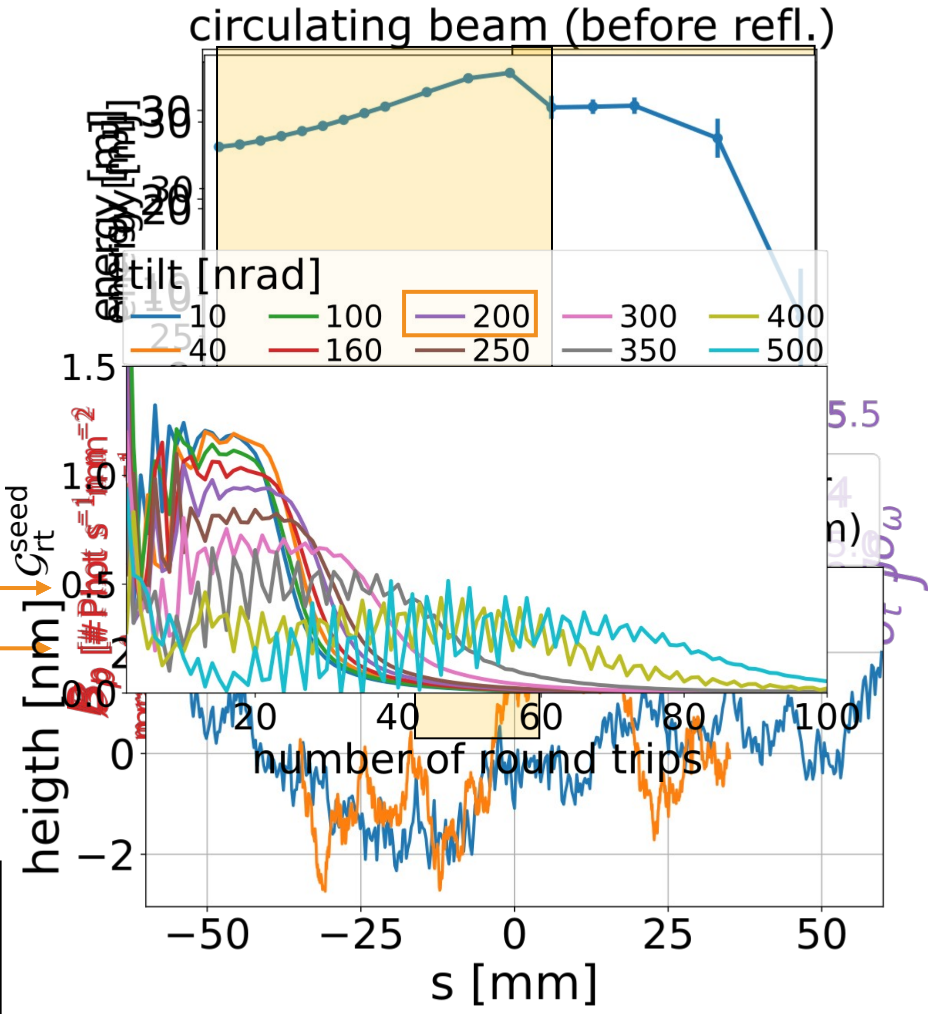
A Cavity Based X-ray FEL Demonstrator at the European XFEL

Non-Idealized Case: What (most relevant) error sources are there?

- Electron beam jitter (shot to shot fluctuations)
  - transverse position jitter (3 µm)
  - pointing jitter (100 nrad)
  - timing jitter (20 fs)
  - beam energy jitter (1.7 MeV) → **reduces stability**

quite robust!

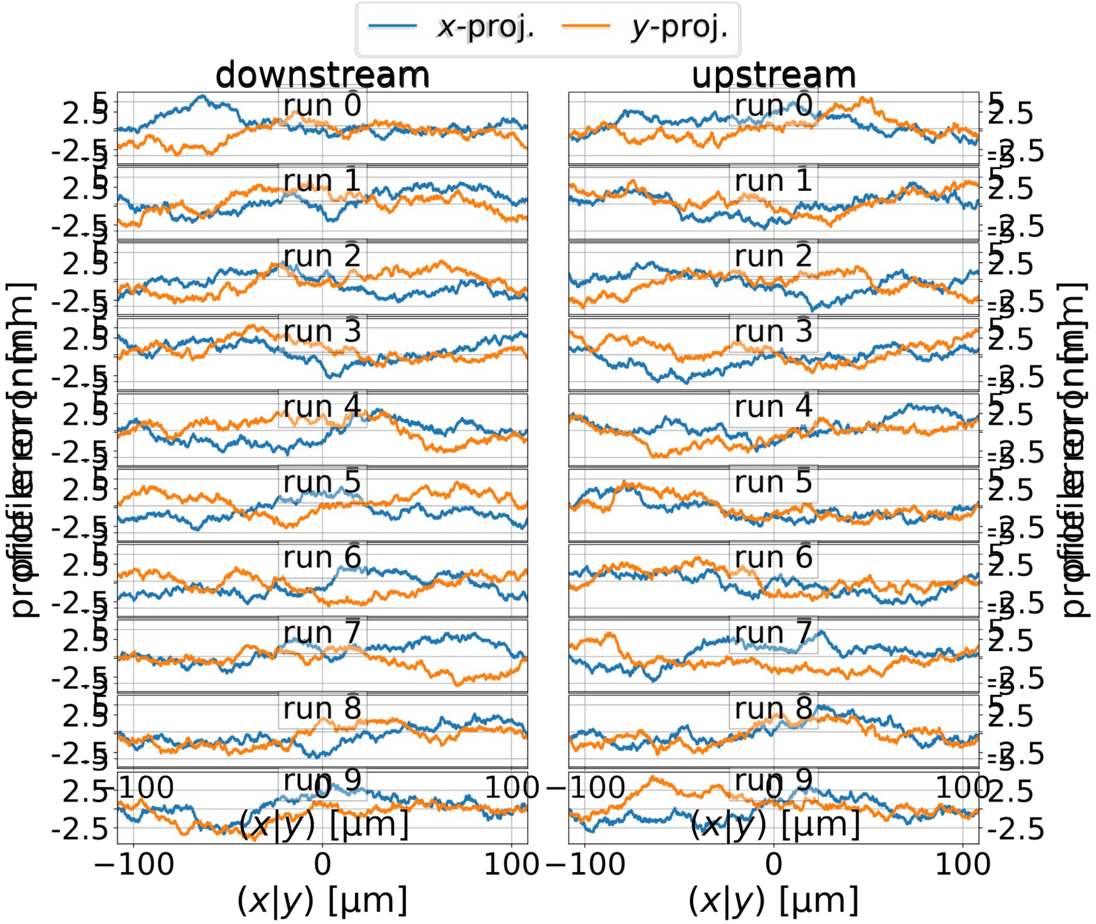
- Optical components
  - Grazing incidence mirror length: 7 cm
  - tilt of crystal: tolerance 00 nrad per crystal
  - Cavity length: tolerance 0 µm → µm
  - Mirror surface error

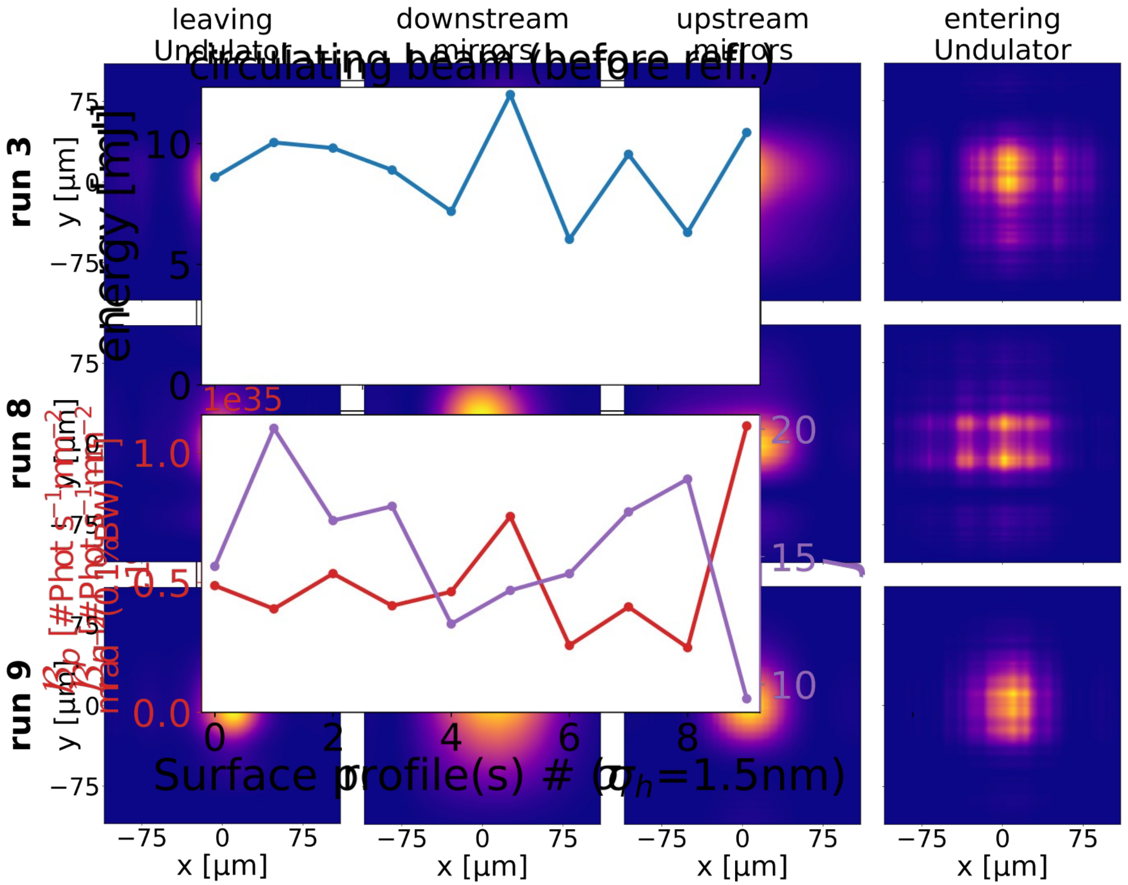


- W. Q. Hua et al., *Using the power spectral density method to characterize and measure the x-ray mirrors surfaces*, Proceeding of 4th IPAC, (2013)

A Cavity Based X-ray FEL Demonstrator at the European XFEL

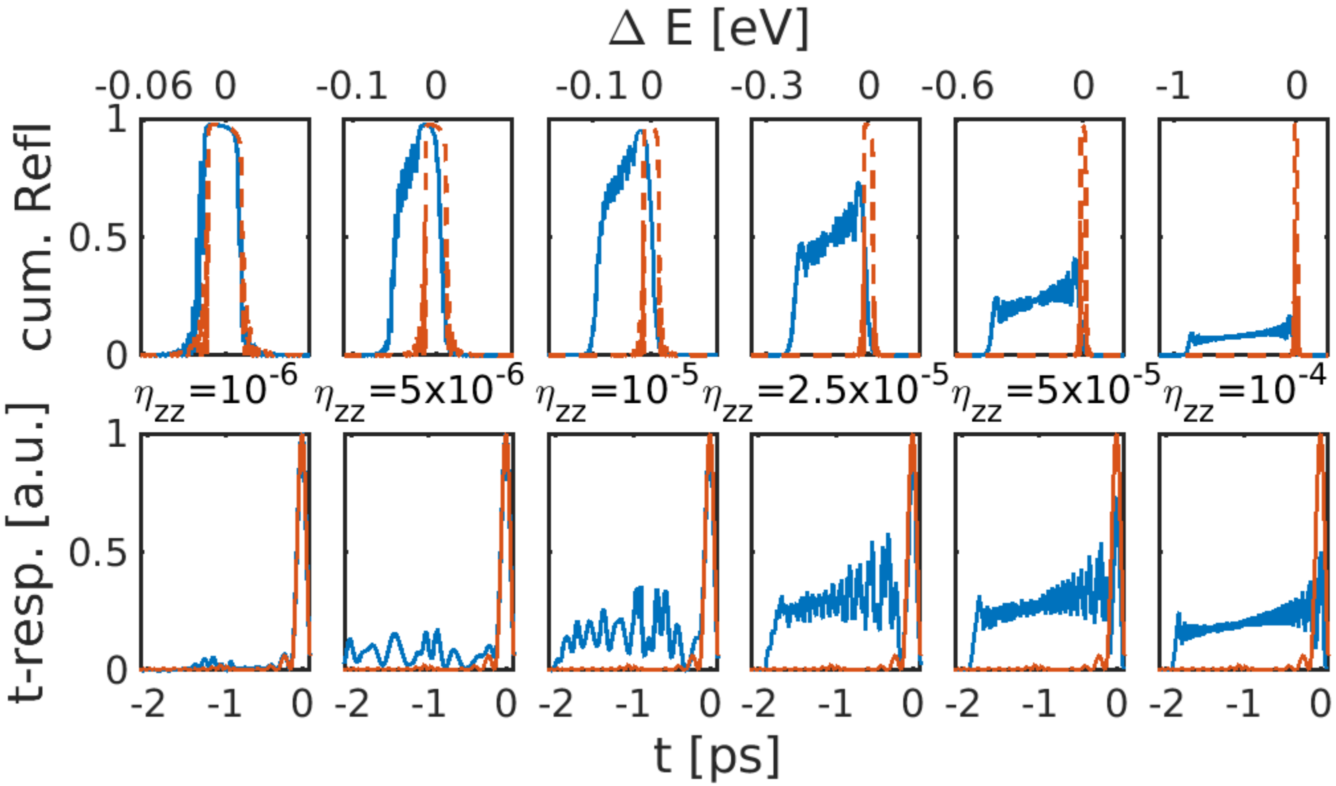
Non-Idealized Case: Mirror Surface Error

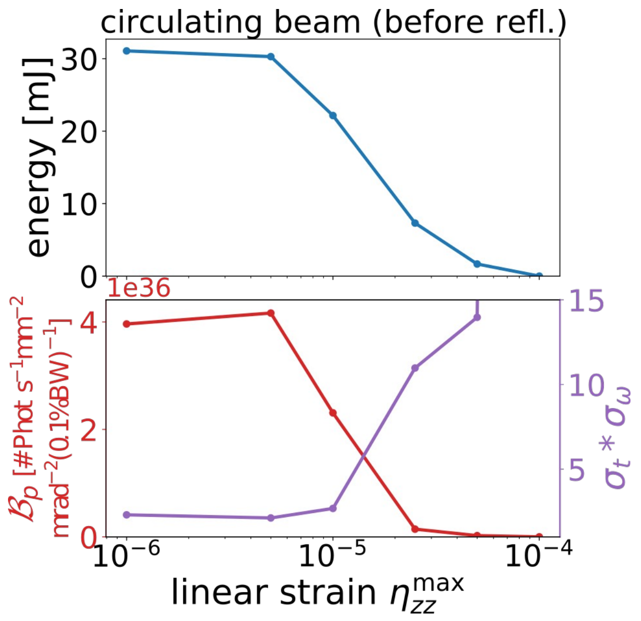


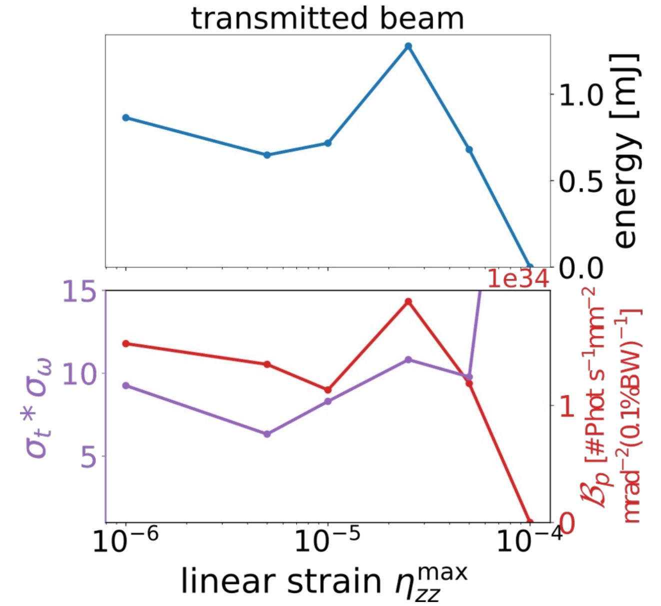


A Cavity Based X-ray FEL Demonstrator at the European XFEL

Non-Idealized Case: Crystal strain







A Cavity Based X-ray FEL Demonstrator at the European XFEL

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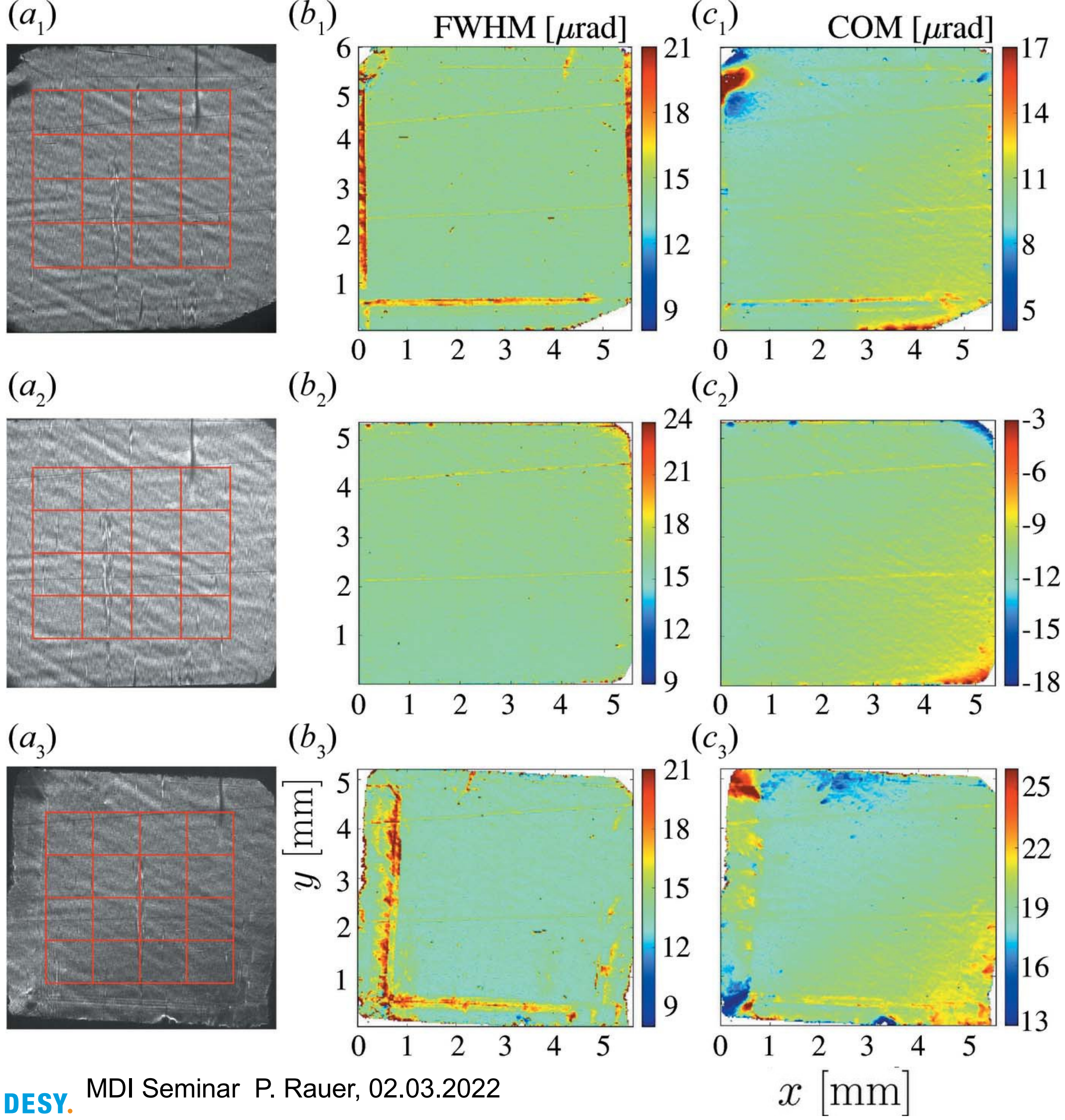
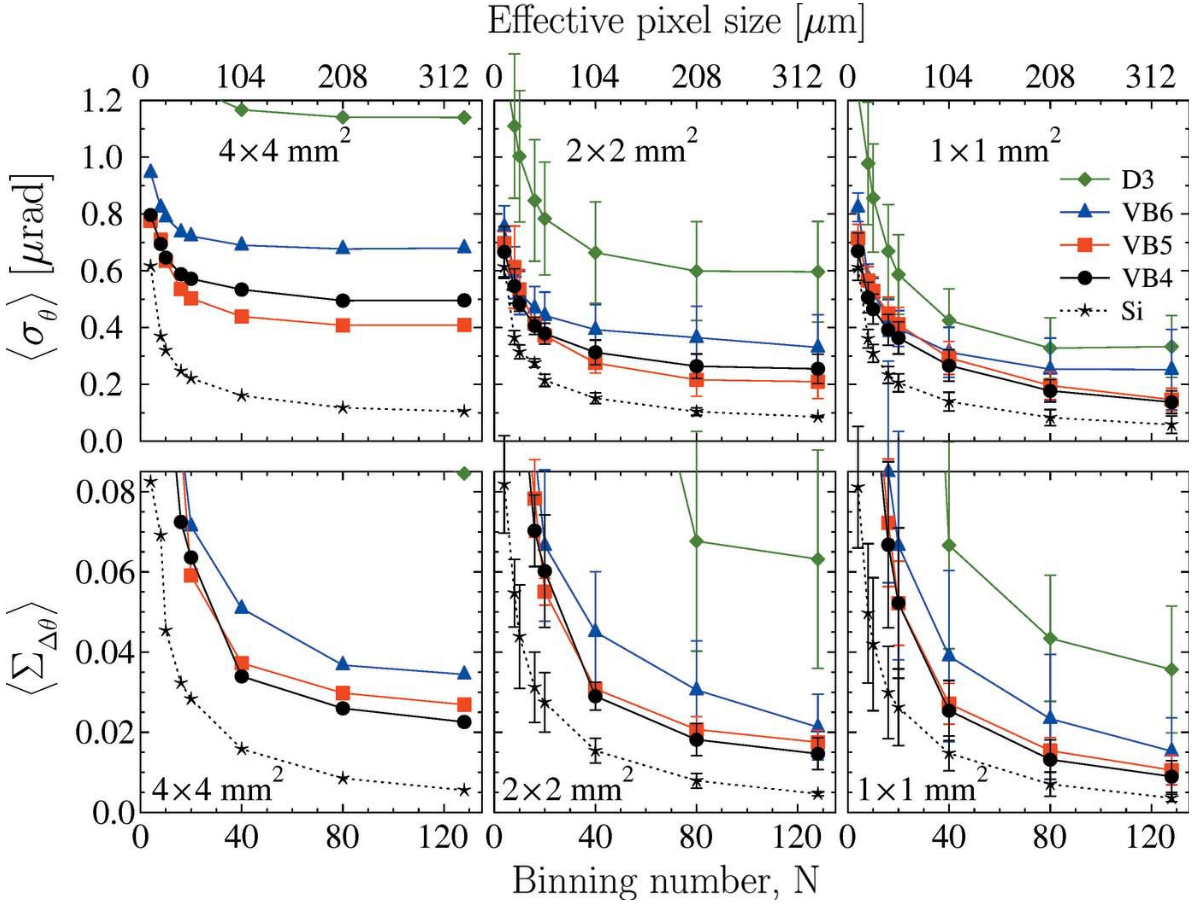
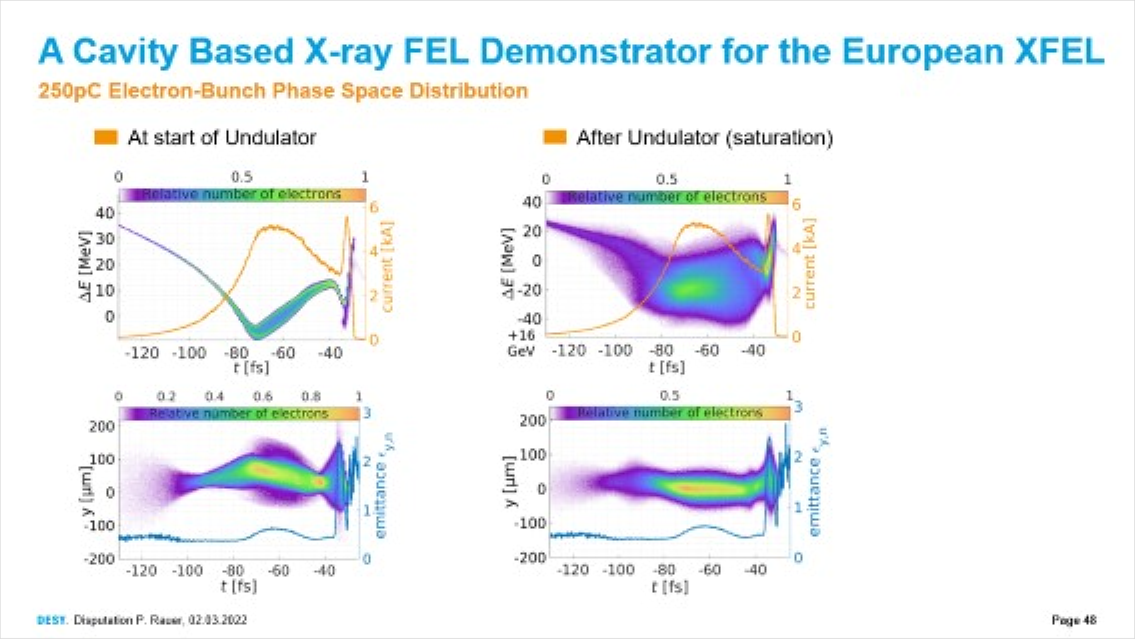




Electron distributions

Electron distribution before and after traversing the undulator



A Cavity Based X-ray FEL Demonstrator for the European XFEL

250pC Electron-Bunch Phase Space Distribution

- At start of Undulator
- After Undulator (saturation)

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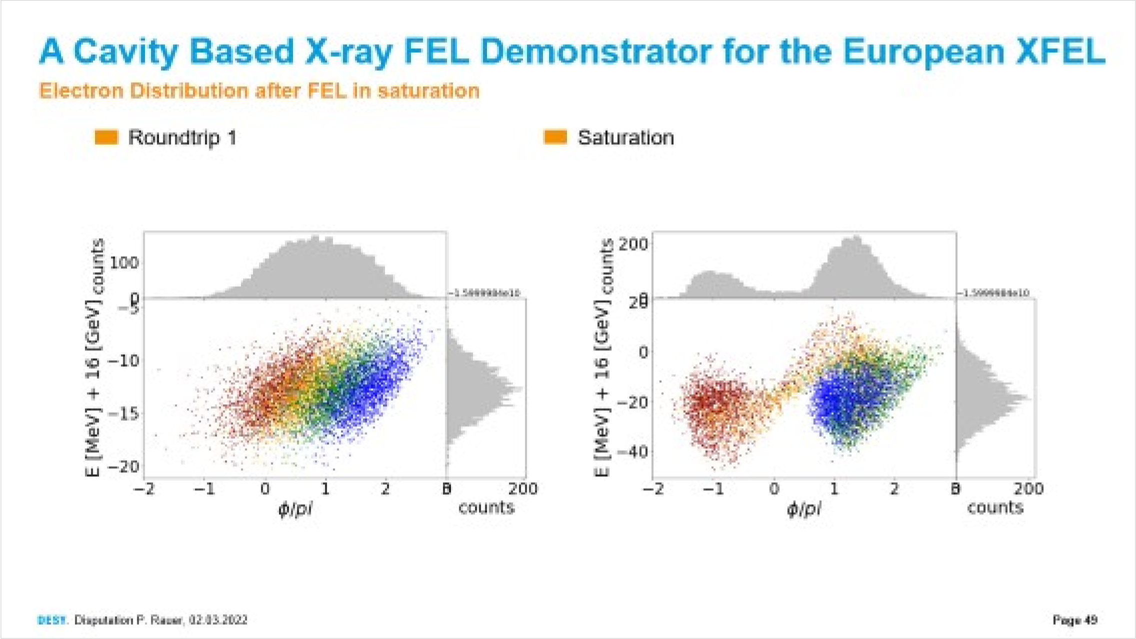

A Cavity Based X-ray FEL Demonstrator for the European XFEL

Electron Distribution after FEL in saturation

- Roundtrip 1
- Saturation

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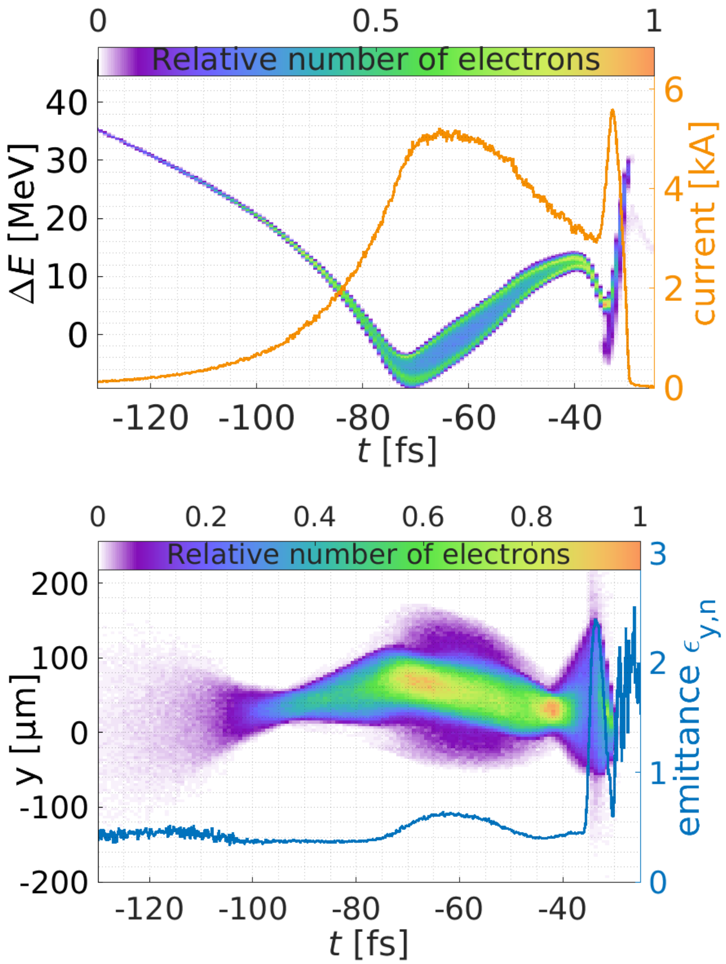
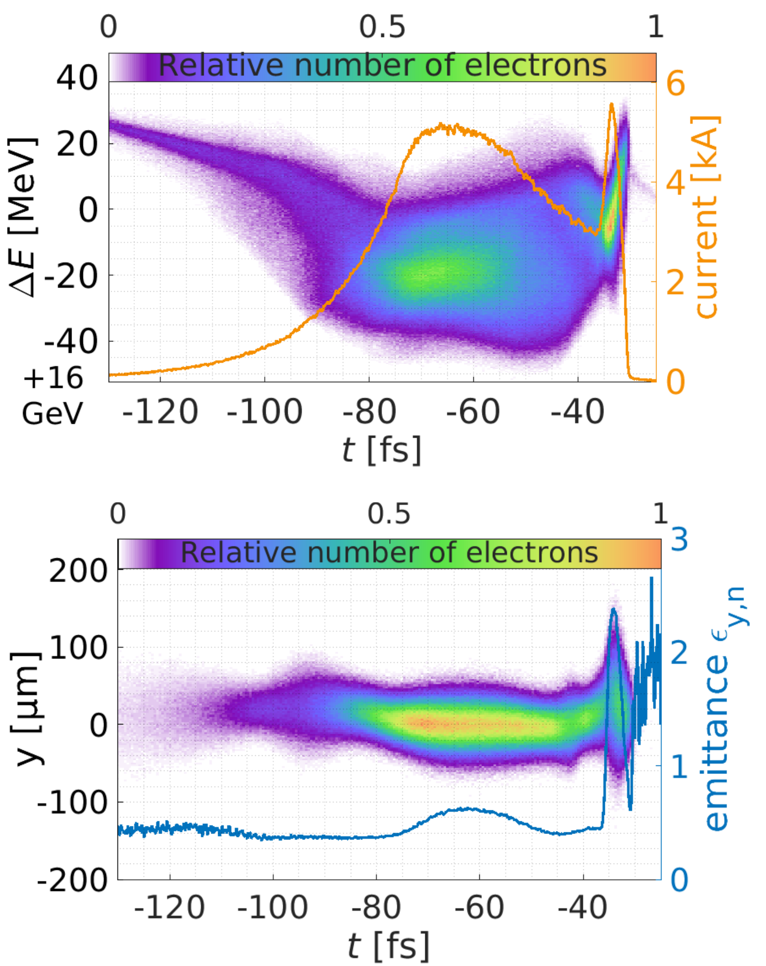
A Cavity Based X-ray FEL Demonstrator for the European XFEL

250pC Electron-Bunch Phase Space Distribution

🟧 At start of Undulator



🟧 After Undulator (saturation)



A Cavity Based X-ray FEL Demonstrator for the European XFEL

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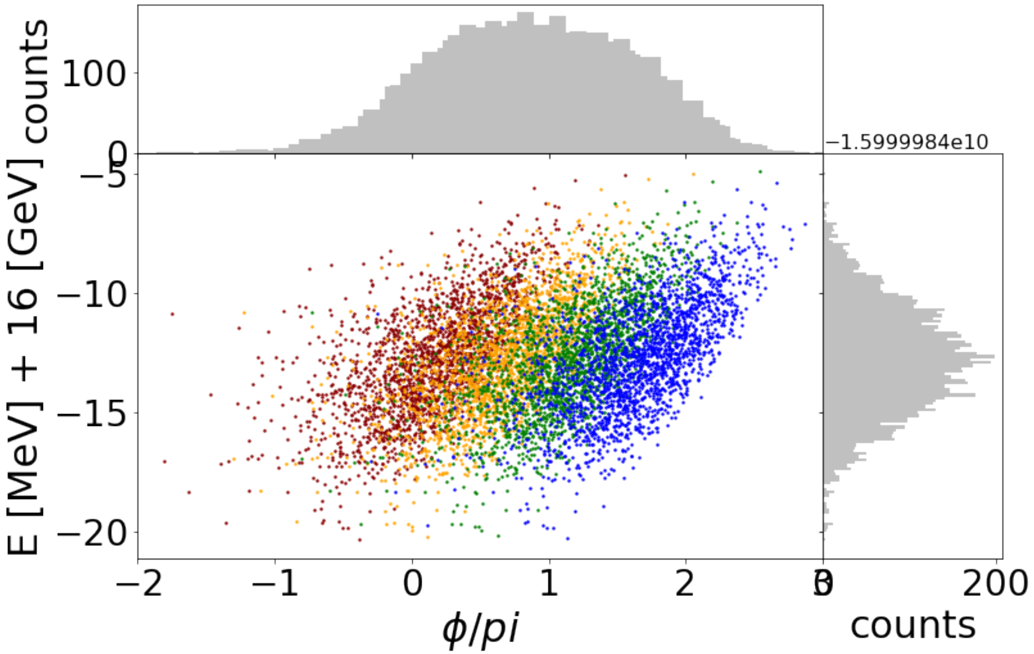
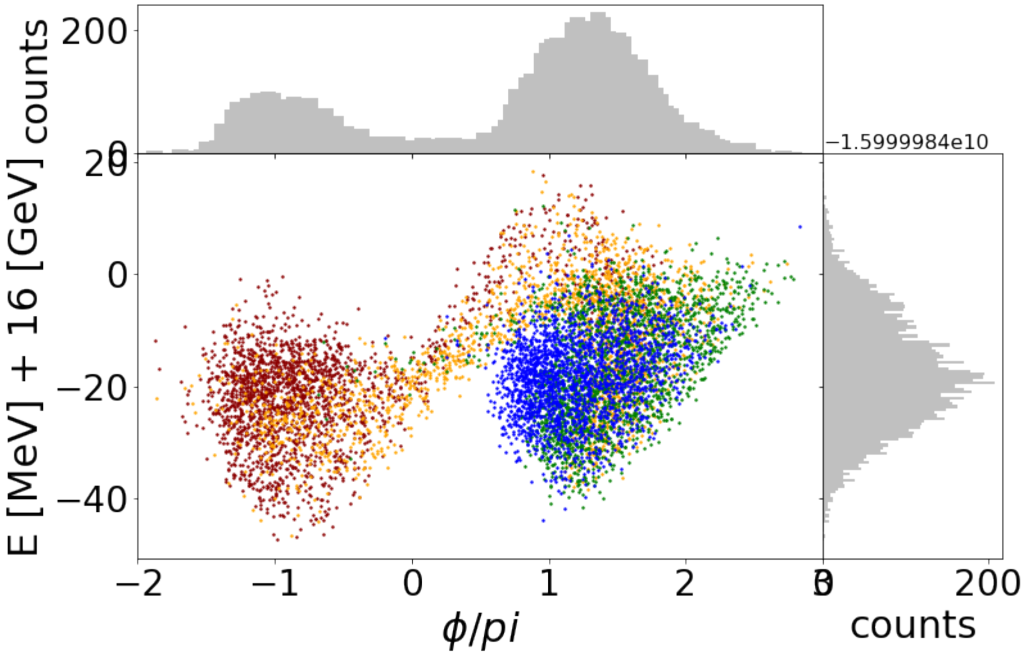


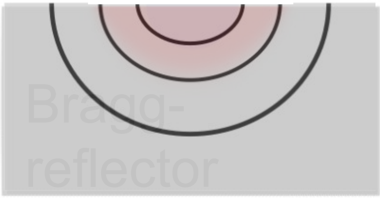
🟧 Saturation



A Cavity Based X-ray FEL Demonstrator at the European XFEL

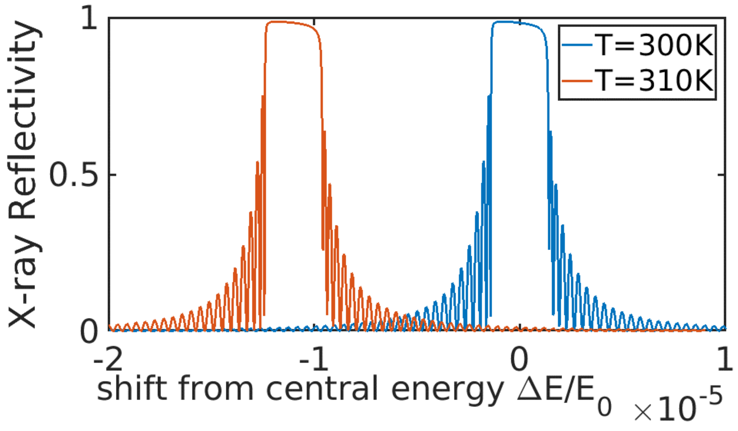
The Problem of Heat Load

- Saturated CBXFEL → ~10 mJ pulse energy incident on crystal at 2 MHz rate
  - Disturbing optical stability (long term vibrations)
  - Disturbing the crystal spectral reflectivity

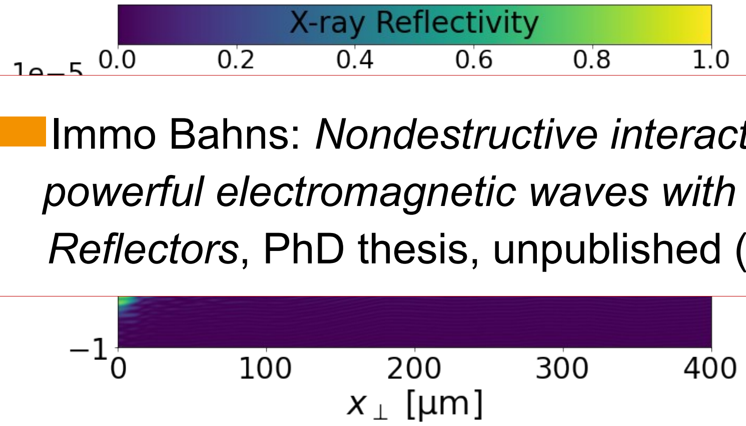


- Lattice thermal expansion (quasistatic)

Implemented



- Dynamic elastic answer of crystal due to rapid thermal expansion after pulse absorption



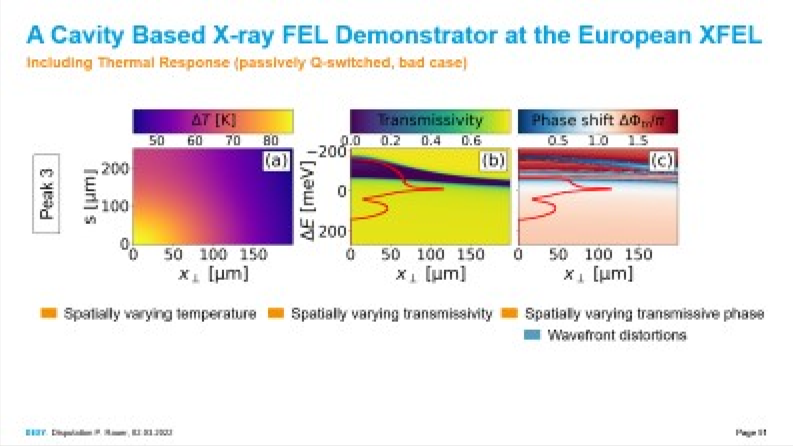
- Immo Bahns: *Nondestructive interaction of powerful electromagnetic waves with Bragg Reflectors*, PhD thesis, unpublished (2022)

ted

Not

Thermal simulations

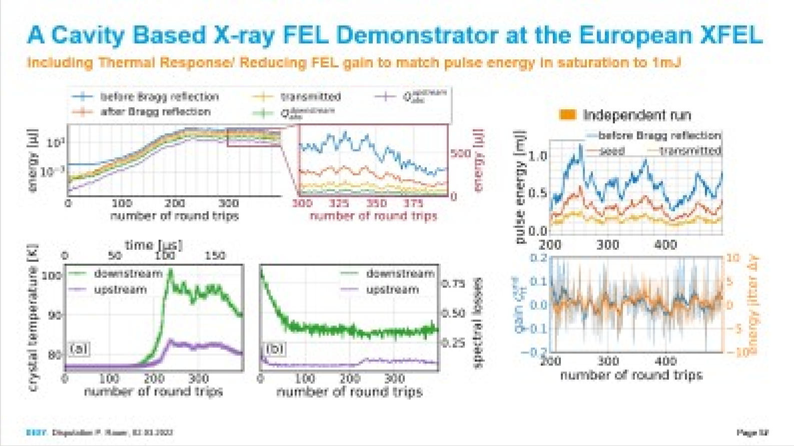
Passively Q-switched, weak gain, impact of thermoelasticity



A Cavity Based X-ray FEL Demonstrator at the European XFEL

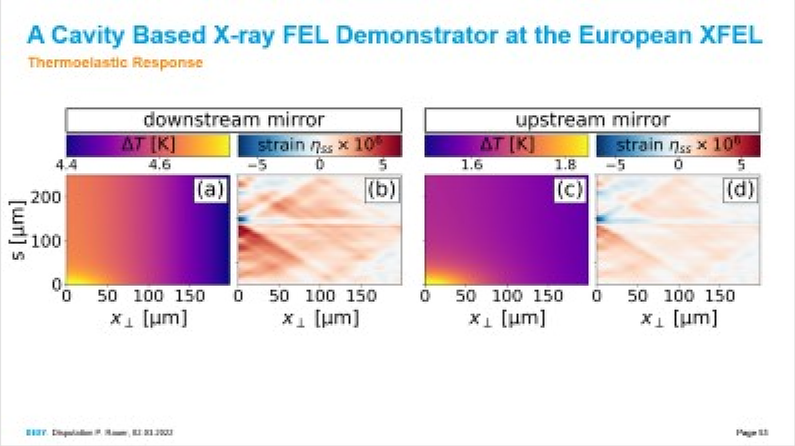
Including Thermal Response (passively Q-switched, bad case)

- 🟧 Spatially varying temperature
- 🟧 Spatially varying transmissivity
- 🟧 Spatially varying transmissive phase
- 🟦 Wavefront distortions



A Cavity Based X-ray FEL Demonstrator at the European XFEL

Including Thermal Response/ Reducing FEL gain to match pulse energy in saturation to 1mJ

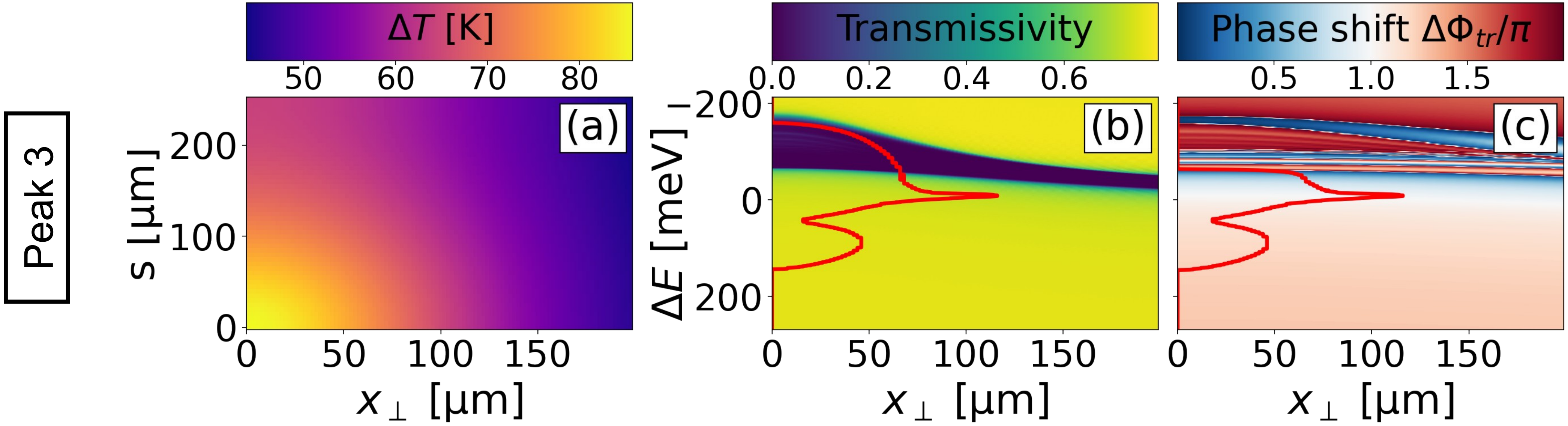


A Cavity Based X-ray FEL Demonstrator at the European XFEL

Thermoelastic Response

A Cavity Based X-ray FEL Demonstrator at the European XFEL

Including Thermal Response (passively Q-switched, bad case)



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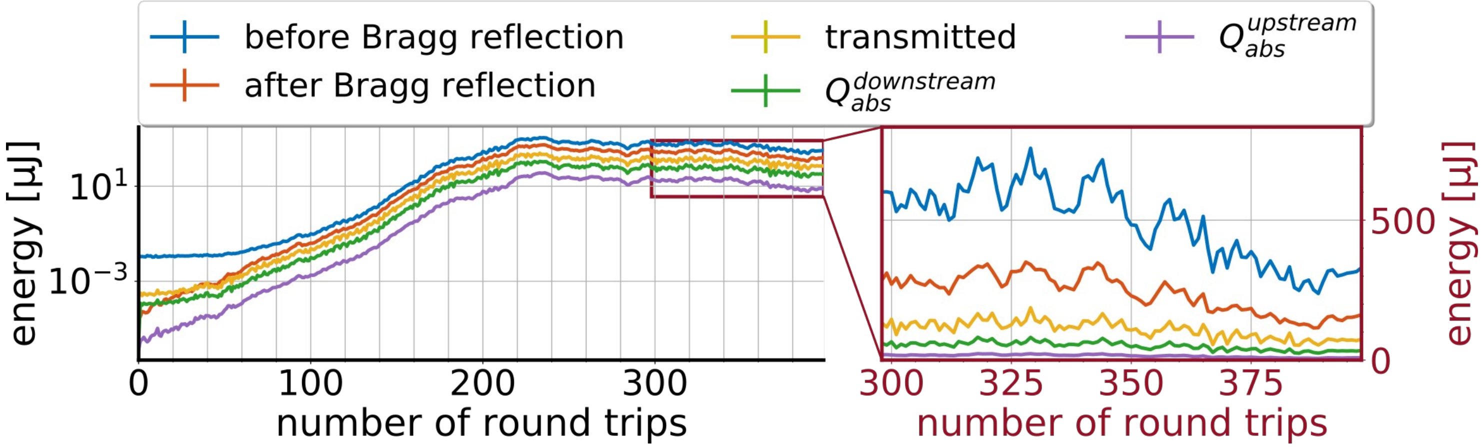
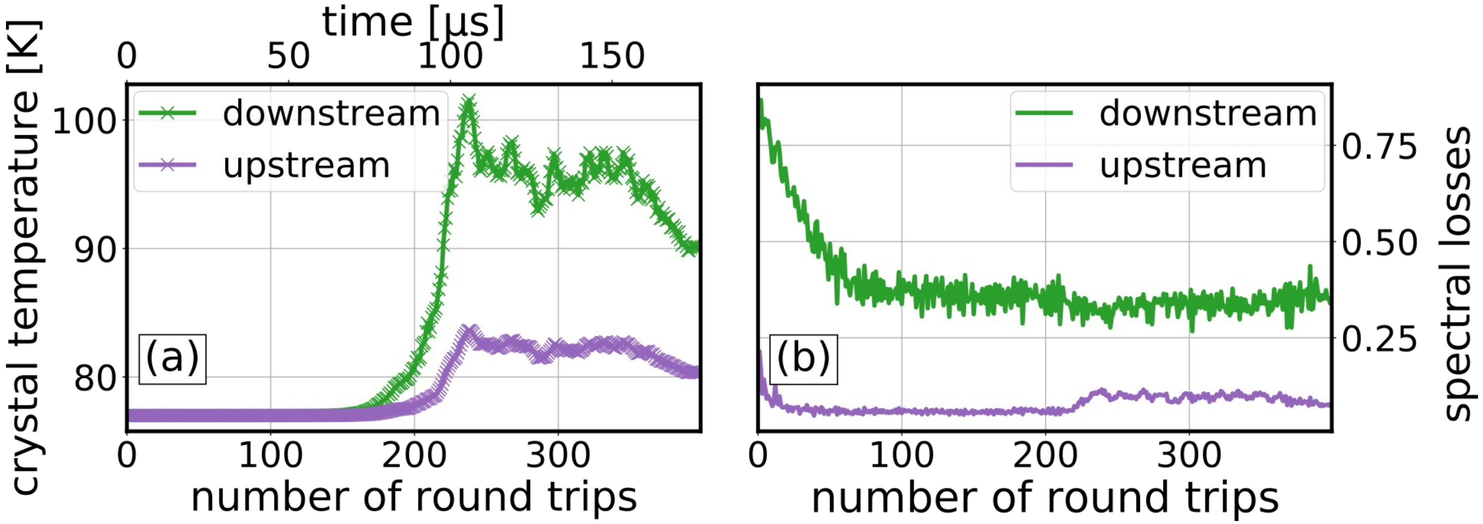
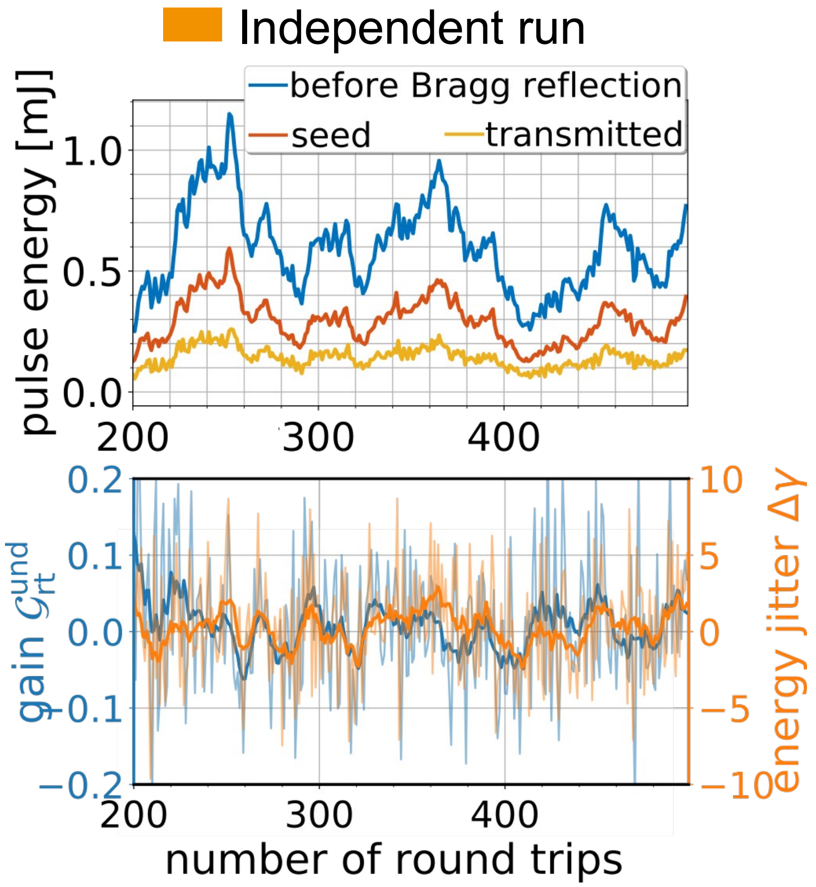
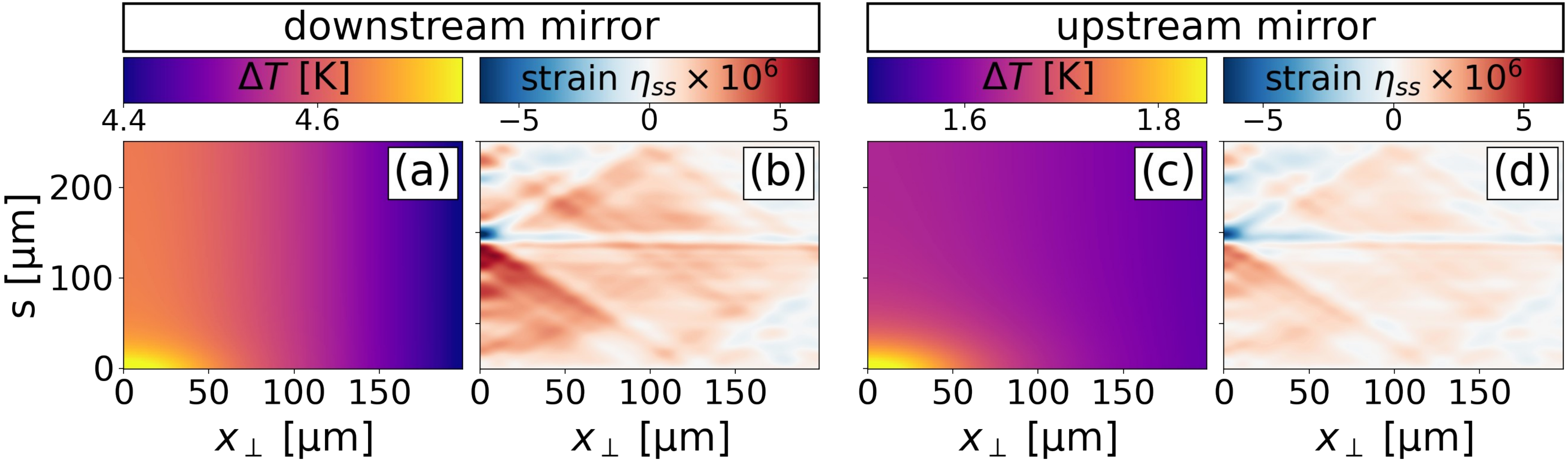






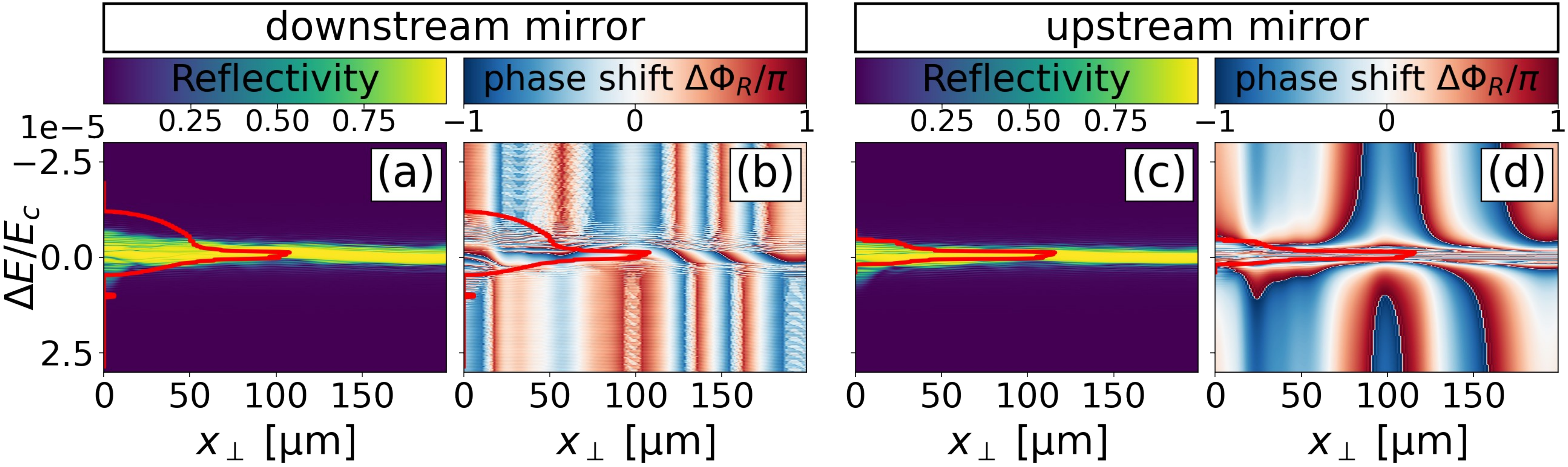
A Cavity Based X-ray FEL Demonstrator at the European XFEL

Thermoelastic Response



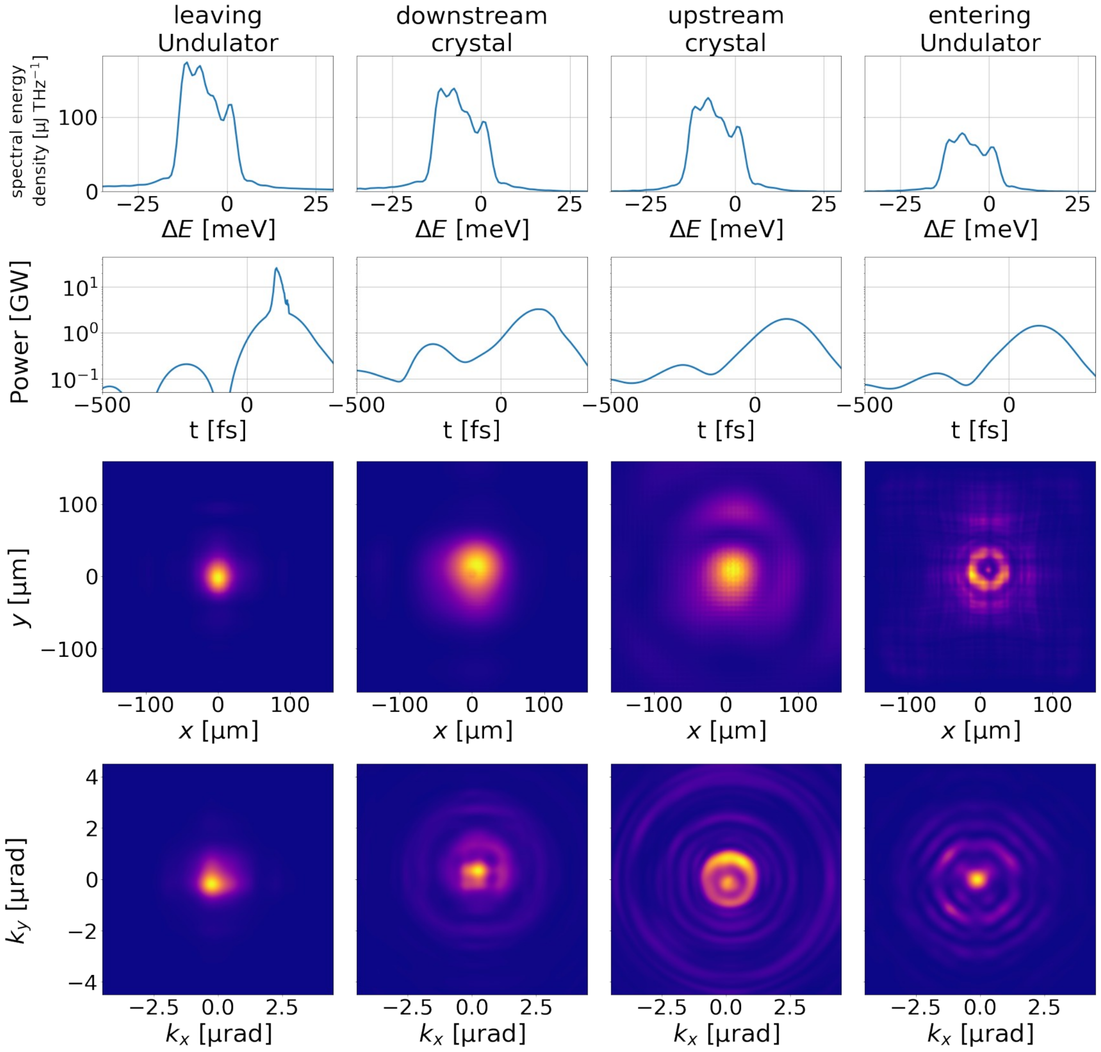
A Cavity Based X-ray FEL Demonstrator at the European XFEL

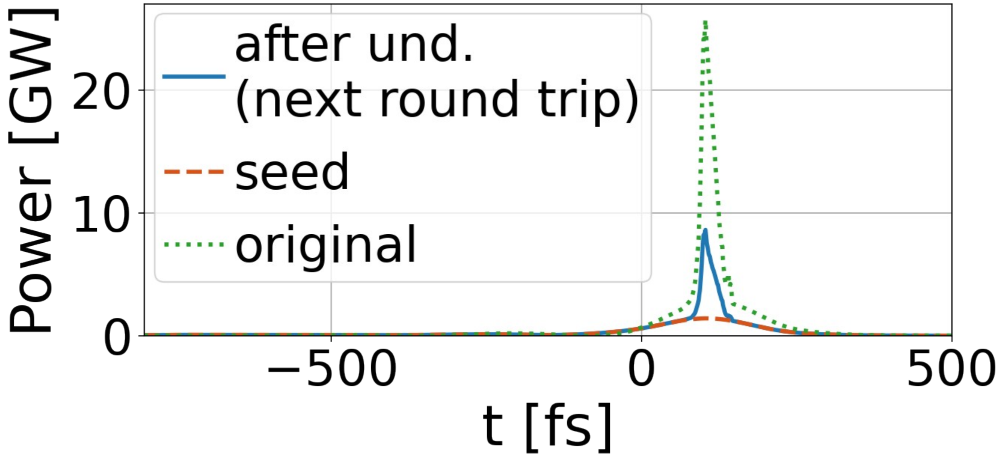
Thermoelastic Response



A Cavity Based X-ray FEL Demonstrator at the European XFEL

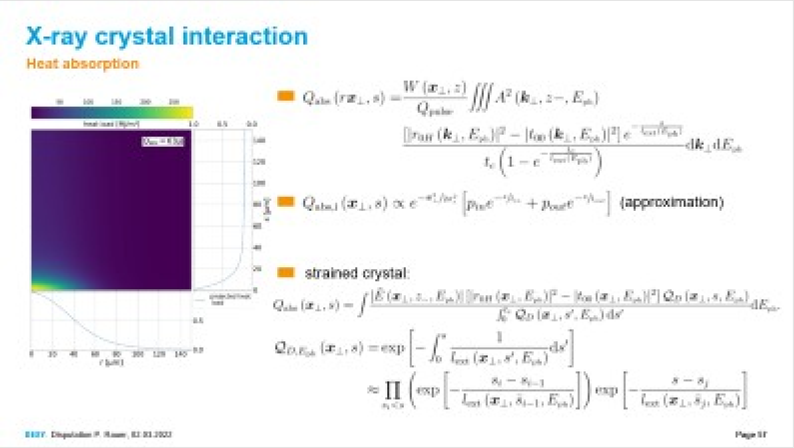
Thermoelastic Response





Background on thermal response

Heatload distribution + advantage of low T + boundary scattering + reduced + size of heat source + diamond probs



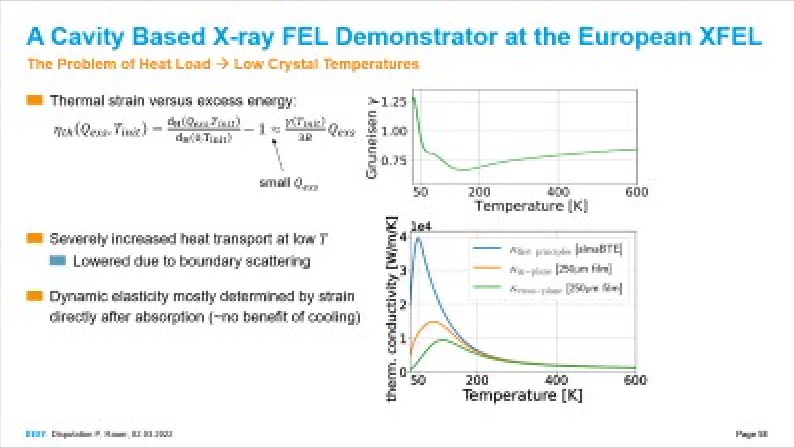
X-ray crystal interaction

Heat absorption

- $Q_{\rm abs}(r\boldsymbol{x}_\perp, s) = \frac{W(\boldsymbol{x}_\perp, z)}{Q_{\rm pulse}} \iiint A^2(\boldsymbol{k}_\perp, z-, E_{ph}) \frac{\left[|r_{0H}(\boldsymbol{k}_\perp,E_{ph})|^2 - |t_{00}(\boldsymbol{k}_\perp,E_{ph})|^2\right] e^{-\frac{s}{l_{\rm ext}(E_{ph})}}}{t_c\left(1-e^{-\frac{t_c}{l_{\rm ext}(E_{ph})}}\right)} d\boldsymbol{k}_\perp dE_{ph}$
- $Q_{\rm abs,l}(\boldsymbol{x}_\perp, s) \propto e^{-x_\perp^2/2\sigma_l^2}\left[p_{\rm in}e^{-s/l_{\rm in}} + p_{\rm out}e^{-s/l_{\rm out}}\right]$ (approximation)
- strained crystal:

$$Q_{\rm abs}(\boldsymbol{x}_\perp,s) = \int \frac{|\tilde E(\boldsymbol{x}_\perp,z_-,E_{ph})|\left[|r_{0H}(\boldsymbol{x}_\perp,E_{ph})|^2-|t_{00}(\boldsymbol{x}_\perp,E_{ph})|^2\right] Q_D(\boldsymbol{x}_\perp,s,E_{ph})}{\int_0^{t_c} Q_D(\boldsymbol{x}_\perp,s',E_{ph})\,ds'} dE_{ph}$$

$$Q_{D,E_{ph}}(\boldsymbol{x}_\perp,s) = \exp\left[-\int_0^s \frac{1}{l_{\rm ext}(\boldsymbol{x}_\perp,s',E_{ph})}ds'\right] \approx \prod_{s_i<s}\left(\exp\left[-\frac{s_i-s_{i-1}}{l_{\rm ext}(\boldsymbol{x}_\perp,s_{i-1},E_{ph})}\right]\right)\exp\left[-\frac{s-s_j}{l_{\rm ext}(\boldsymbol{x}_\perp,s_j,E_{ph})}\right]$$



A Cavity Based X-ray FEL Demonstrator at the European XFEL

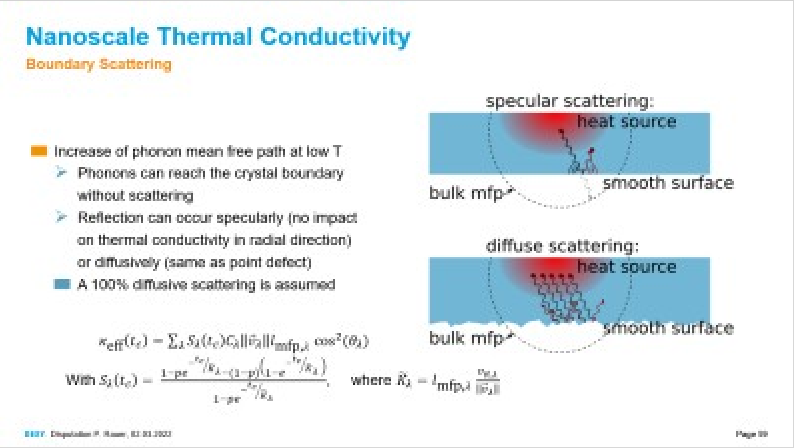
The Problem of Heat Load → Low Crystal Temperatures

- Thermal strain versus excess energy:

$$\eta_{th}(Q_{exs}, T_{init}) = \frac{d_H(Q_{exs}, T_{init})}{d_H(0, T_{init})} - 1 \approx \frac{\gamma(T_{init})}{3B}Q_{exs}$$

small Q_{exs}

- Severely increased heat transport at low T
  - Lowered due to boundary scattering
- Dynamic elasticity mostly determined by strain directly after absorption (~no benefit of cooling)



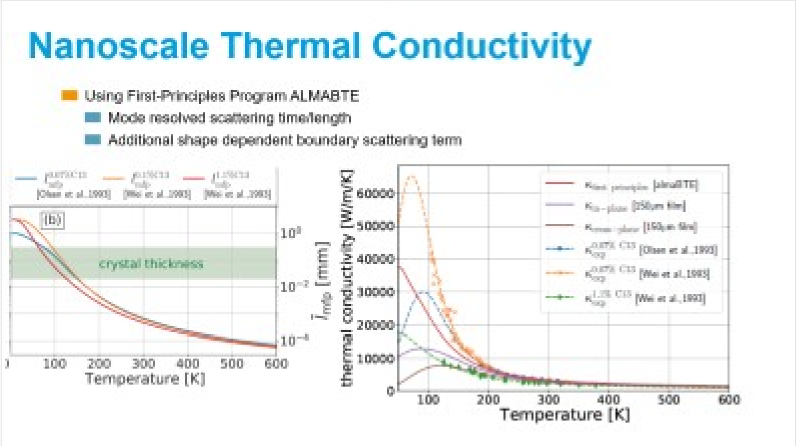
Nanoscale Thermal Conductivity

Boundary Scattering

- Increase of phonon mean free path at low T
  - Phonons can reach the crystal boundary without scattering
  - Reflection can occur specularly (no impact on thermal conductivity in radial direction) or diffusively (same as point defect)
  - A 100% diffusive scattering is assumed

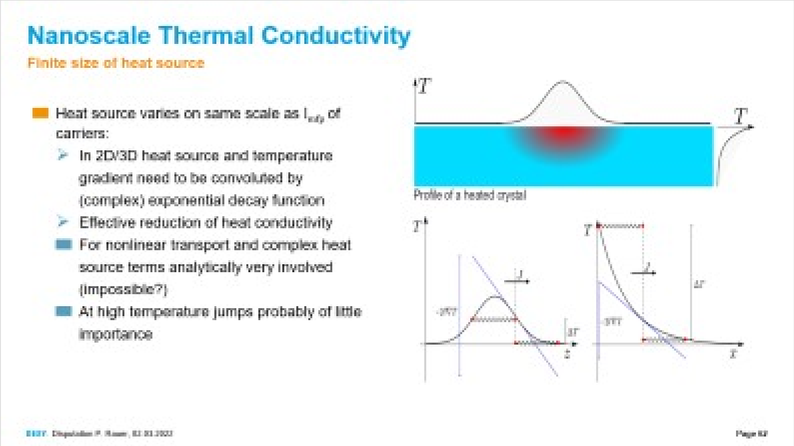
$$\kappa_{\rm eff}(t_c) = \sum_\lambda S_\lambda(t_c)C_\lambda\|\vec v_\lambda\| l_{{\rm mfp},\lambda}\cos^2(\theta_\lambda)$$

With $S_\lambda(t_c) = \frac{1-pe^{-t_c/K_\lambda}-(1-p)\left(1-e^{-t_c/K_\lambda}\right)}{1-pe^{-t_c/K_\lambda}}$, where $K_\lambda = l_{{\rm mfp},\lambda}\frac{v_{z,\lambda}}{\|\vec v_\lambda\|}$



Nanoscale Thermal Conductivity

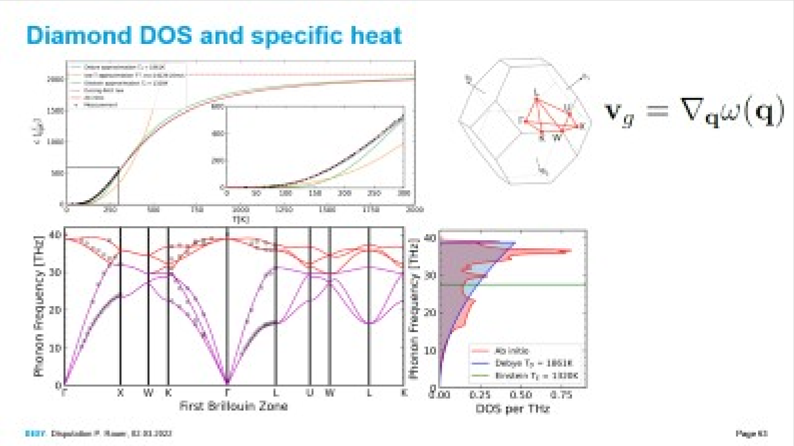
- Using First-Principles Program ALMABTE
  - Mode resolved scattering time/length
  - Additional shape dependent boundary scattering term



Nanoscale Thermal Conductivity

Finite size of heat source

- Heat source varies on same scale as l_{mfp} of carriers:
  - In 2D/3D heat source and temperature gradient need to be convoluted by (complex) exponential decay function
  - Effective reduction of heat conductivity
  - For nonlinear transport and complex heat source terms analytically very involved (impossible?)
  - At high temperature jumps probably of little importance

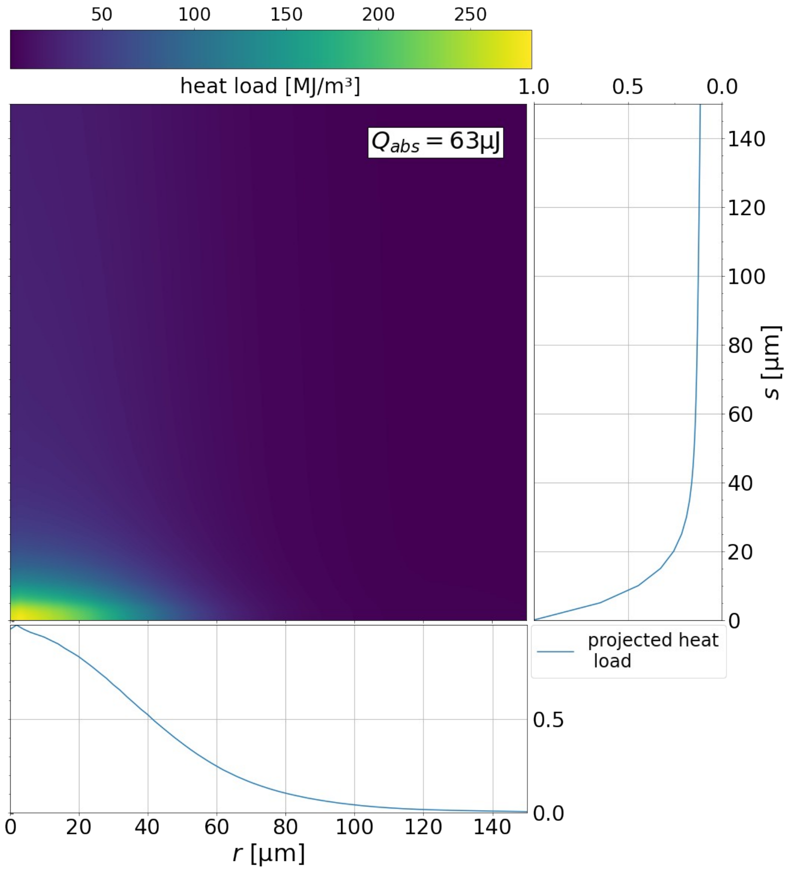


Diamond DOS and specific heat

$$\mathbf{v}_g = \nabla_{\mathbf{q}}\omega(\mathbf{q})$$

X-ray crystal interaction

Heat absorption



- $$Q_{\rm abs}\left(r\boldsymbol{x}_\perp, s\right) = \frac{W\left(\boldsymbol{x}_\perp, z\right)}{Q_{\rm pulse}} \iiint A^2\left(\boldsymbol{k}_\perp, z-, E_{\rm ph}\right) \frac{\left[\left|r_{0H}\left(\boldsymbol{k}_\perp, E_{\rm ph}\right)\right|^2 - \left|t_{00}\left(\boldsymbol{k}_\perp, E_{\rm ph}\right)\right|^2\right] e^{-\frac{s}{l_{\rm ext}(E_{\rm ph})}}}{t_c\left(1 - e^{-\frac{t_c}{l_{\rm ext}(E_{\rm ph})}}\right)} \mathrm{d}\boldsymbol{k}_\perp \mathrm{d}E_{\rm ph}$$

- $$Q_{\rm abs,i}\left(\boldsymbol{x}_\perp, s\right) \propto e^{-\boldsymbol{x}_\perp^2/2\sigma_r^2}\left[p_{in}e^{-s/l_{in}} + p_{out}e^{-s/l_{out}}\right]$$ (approximation)

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$$\mathcal{Q}_{D,E_{\rm ph}}\left(\boldsymbol{x}_\perp, s\right) = \exp\left[-\int_0^s \frac{1}{l_{\rm ext}\left(\boldsymbol{x}_\perp, s', E_{\rm ph}\right)}\mathrm{d}s'\right]$$

$$\approx \prod_{s_i<s}\left(\exp\left[-\frac{s_i - s_{i-1}}{l_{\rm ext}\left(\boldsymbol{x}_\perp, \bar{s}_{i-1}, E_{\rm ph}\right)}\right]\right) \exp\left[-\frac{s - s_j}{l_{\rm ext}\left(\boldsymbol{x}_\perp, \bar{s}_j, E_{\rm ph}\right)}\right]$$

A Cavity Based X-ray FEL Demonstrator at the European XFEL

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  - Lowered due to boundary scattering
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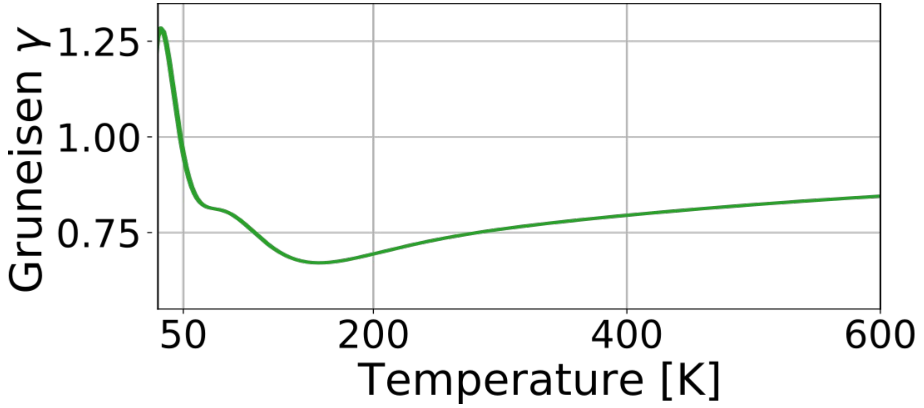

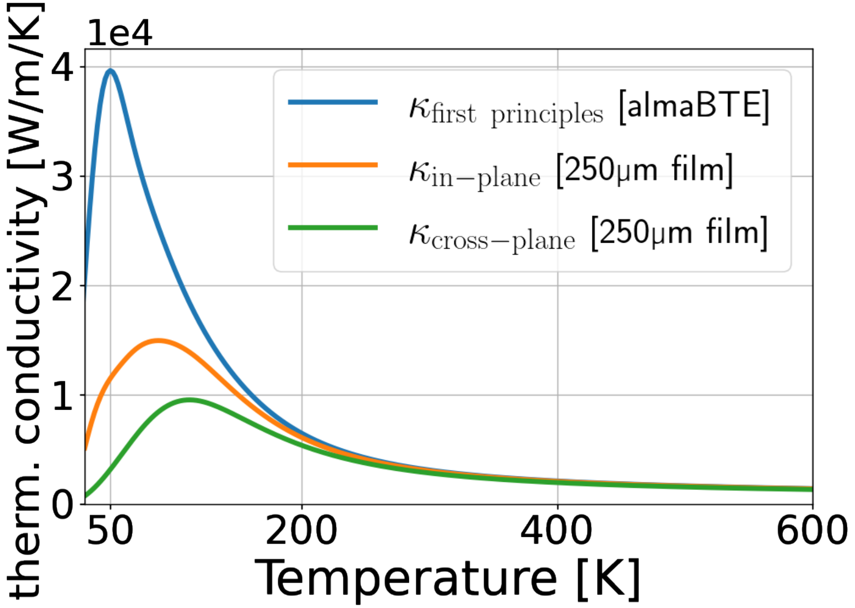

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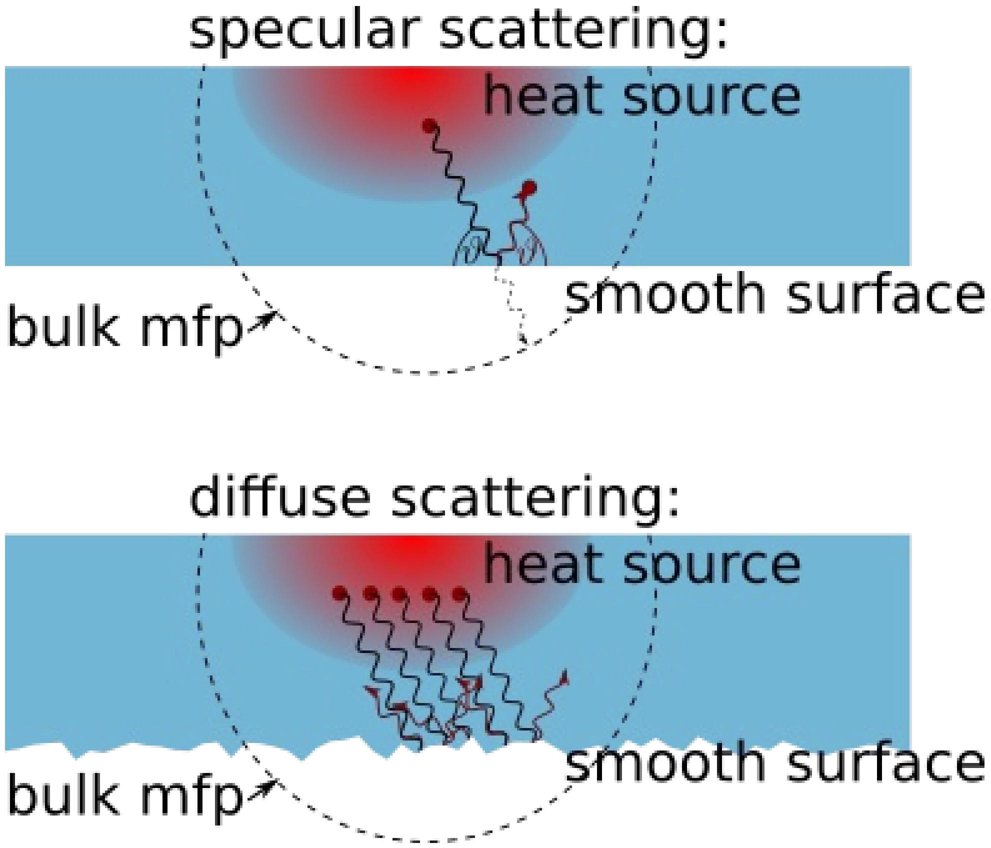
With , where



Nanoscale Thermal Conductivity

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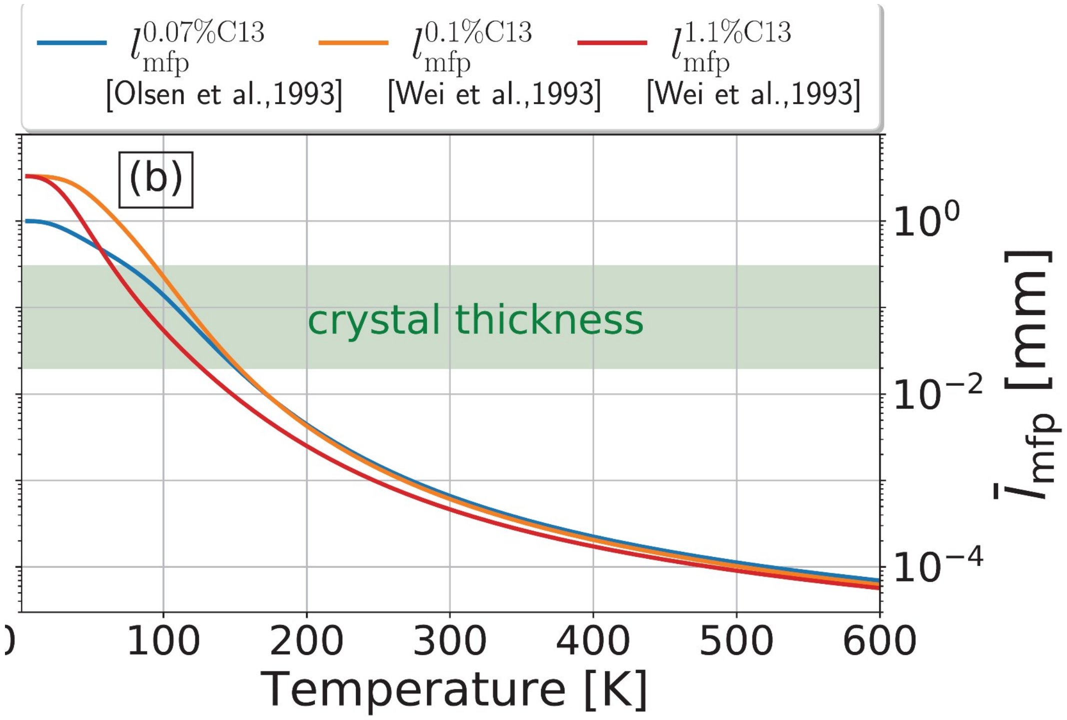

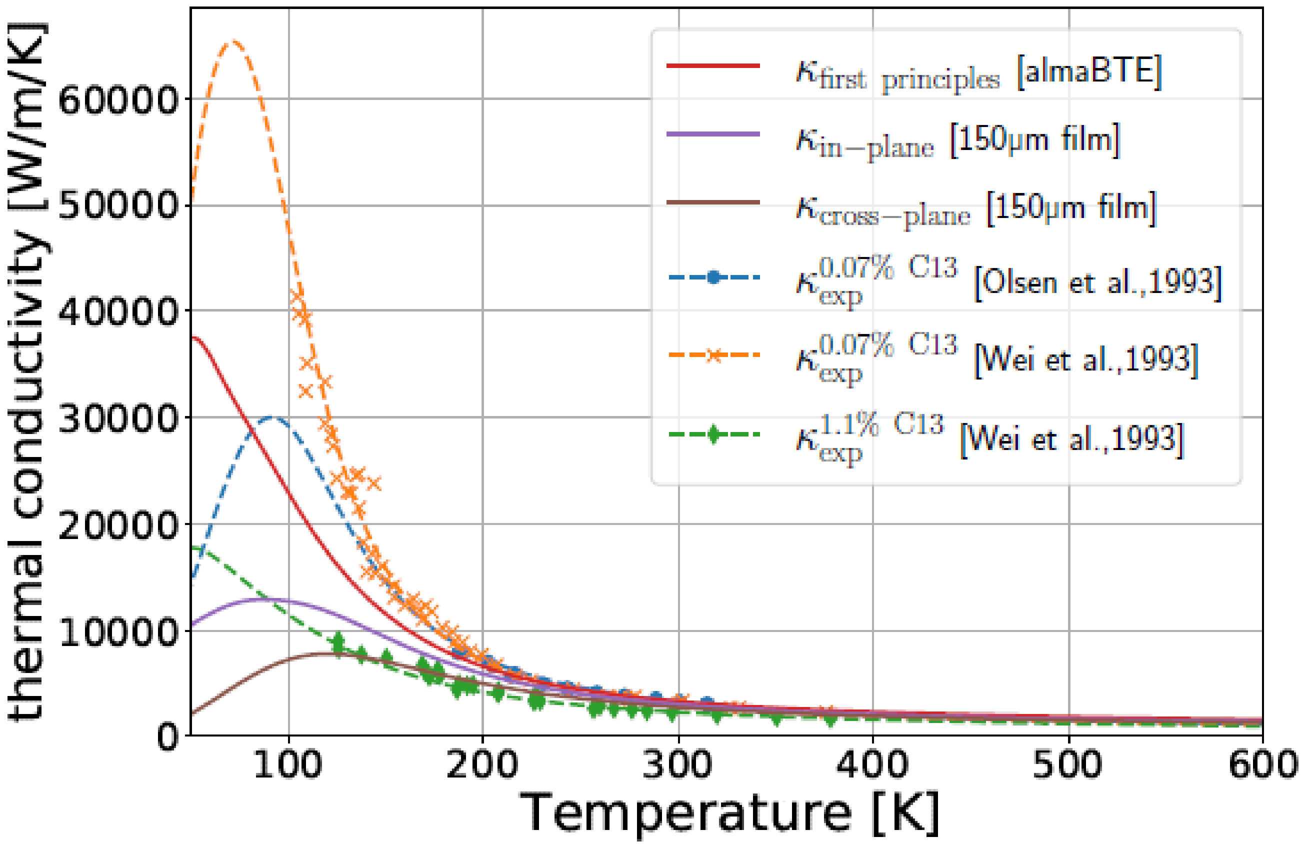

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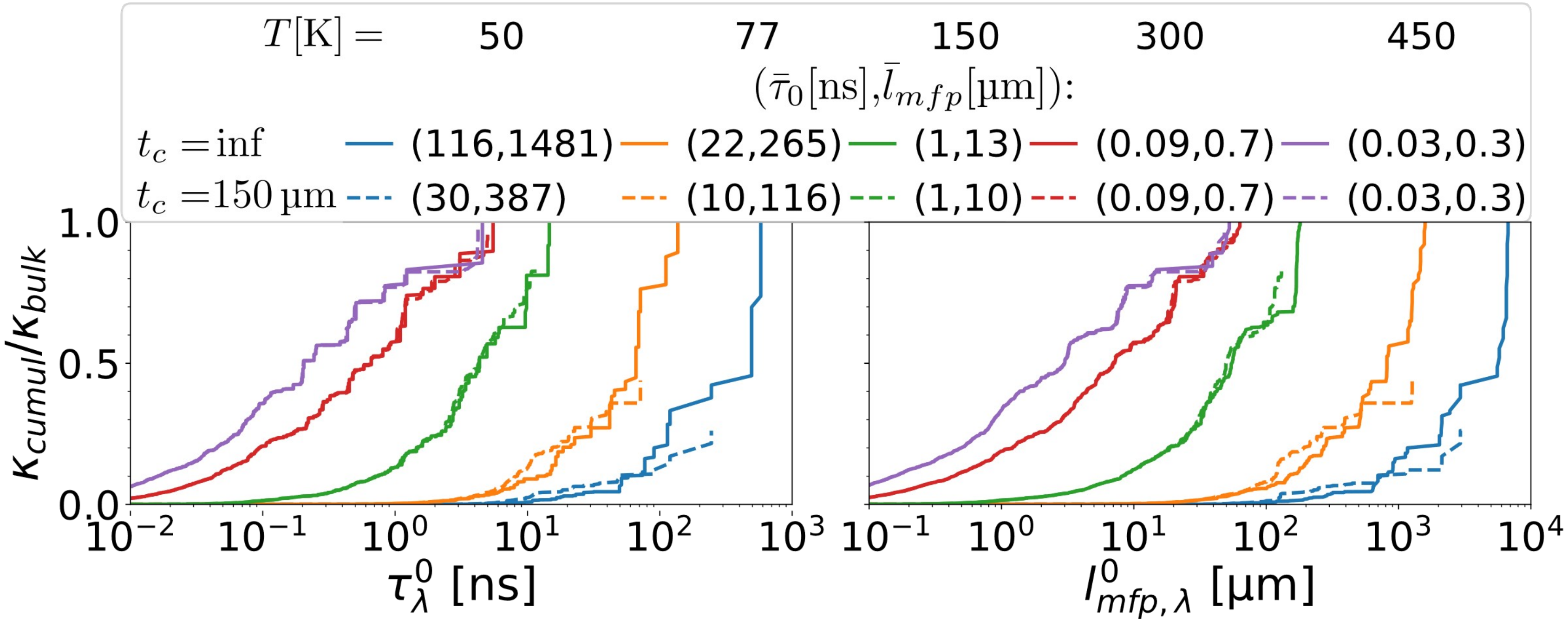

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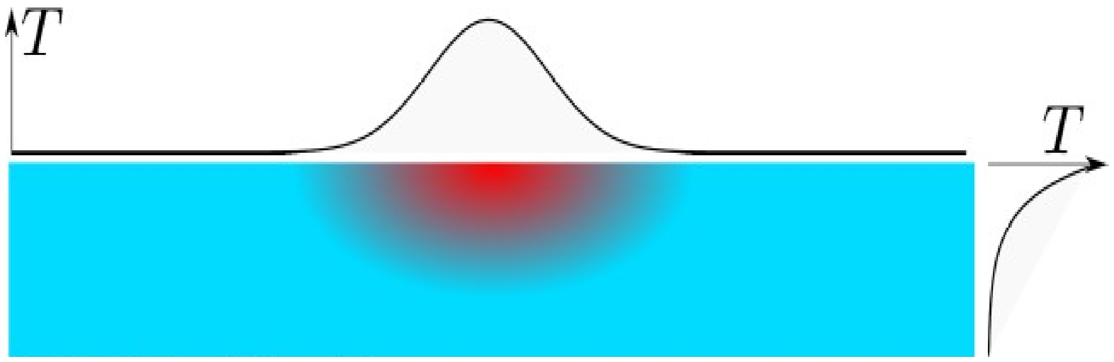
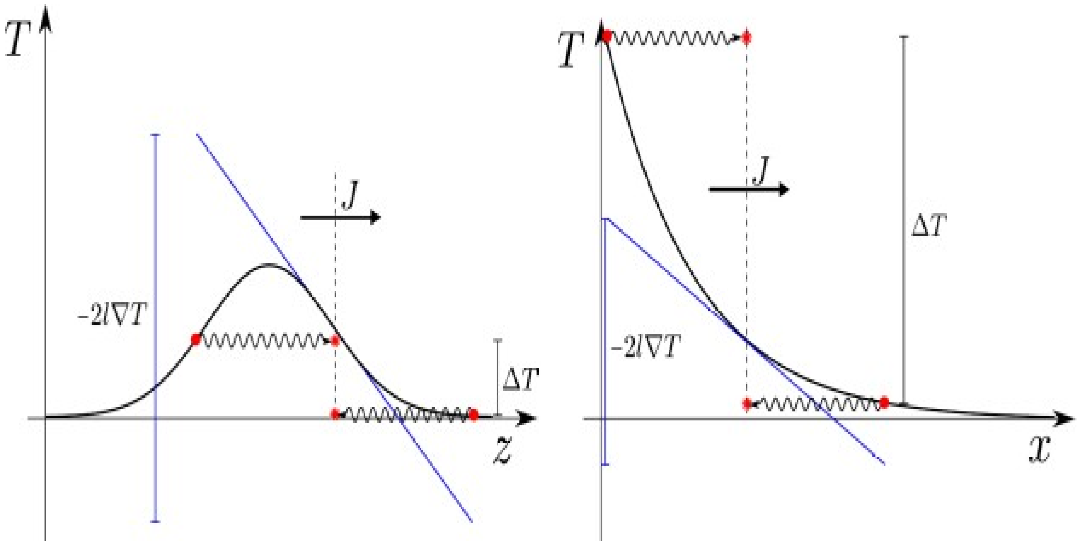
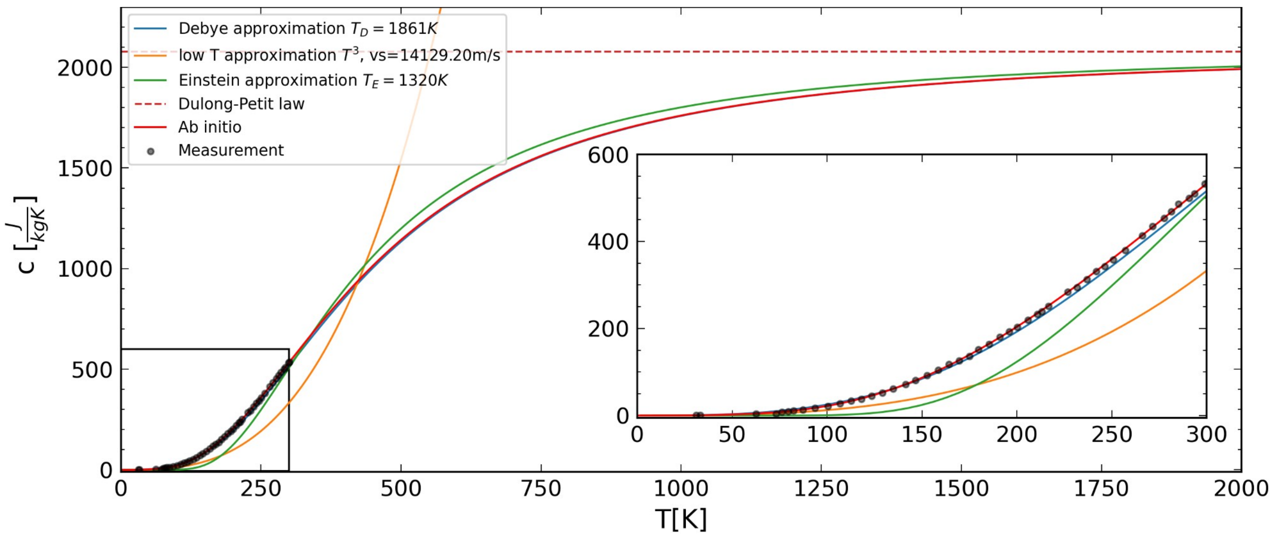
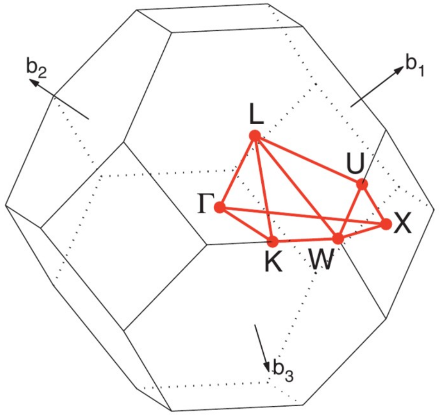


Profile of a heated crystal

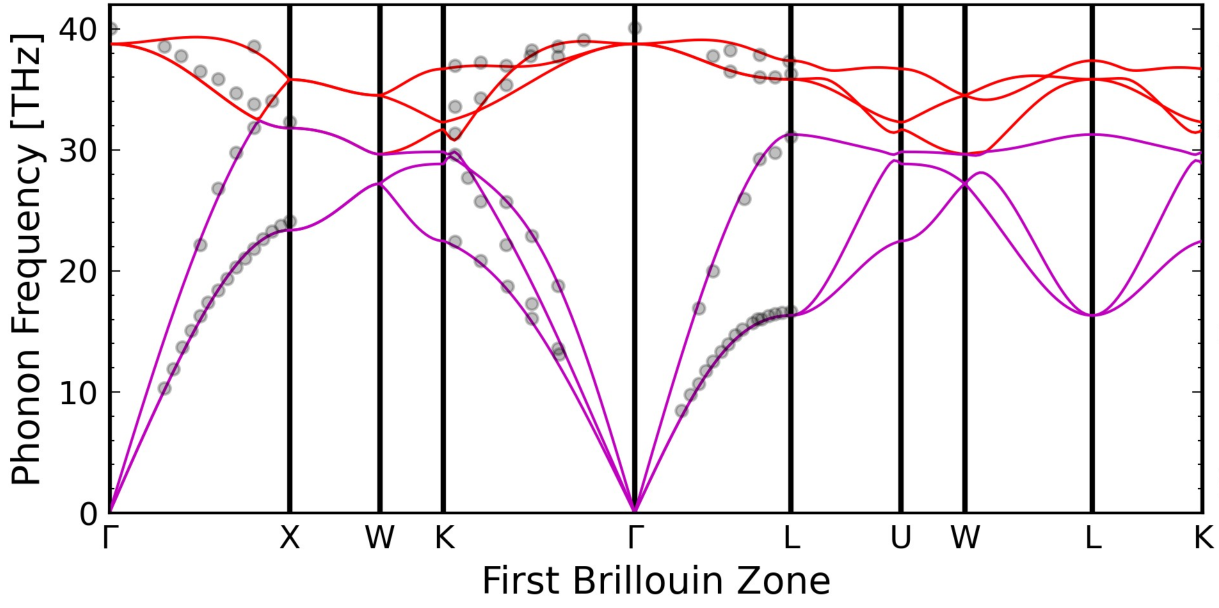


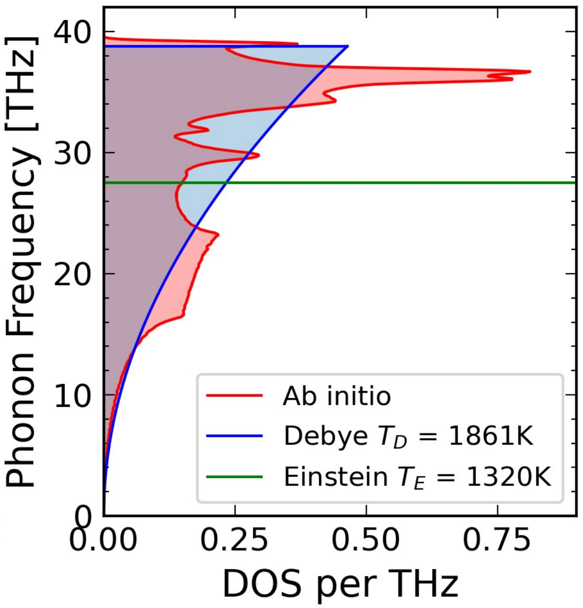
Diamond DOS and specific heat





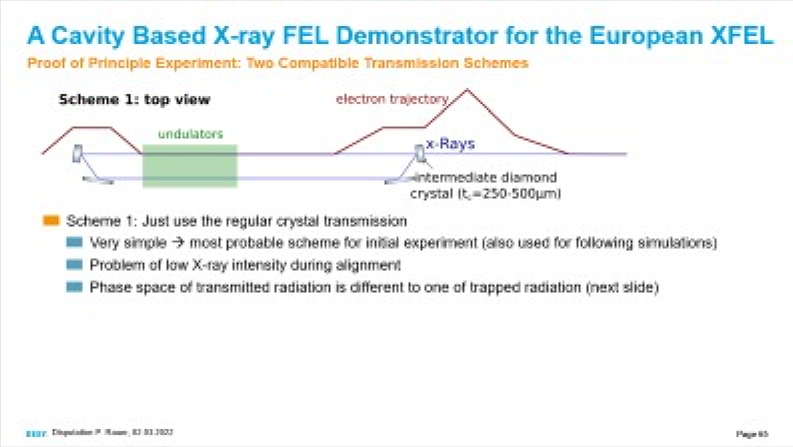
$$\mathbf{v}_g = \nabla_{\mathbf{q}}\omega(\mathbf{q})$$





Alignment

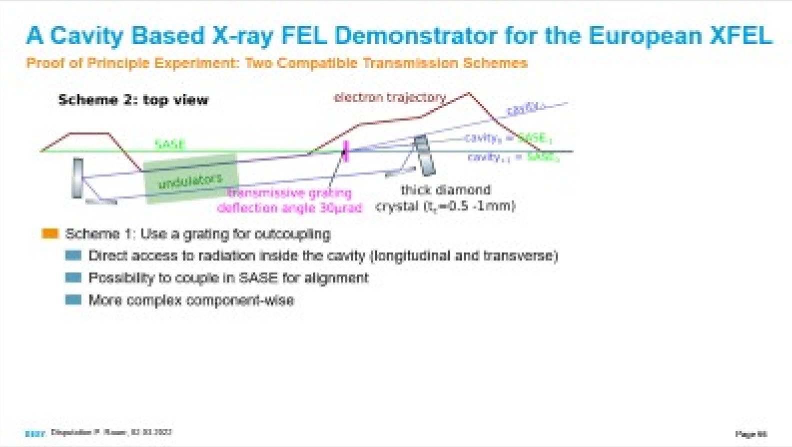
Crystal transmission scheme + Grating scheme + step by step alignment



A Cavity Based X-ray FEL Demonstrator for the European XFEL

Proof of Principle Experiment: Two Compatible Transmission Schemes

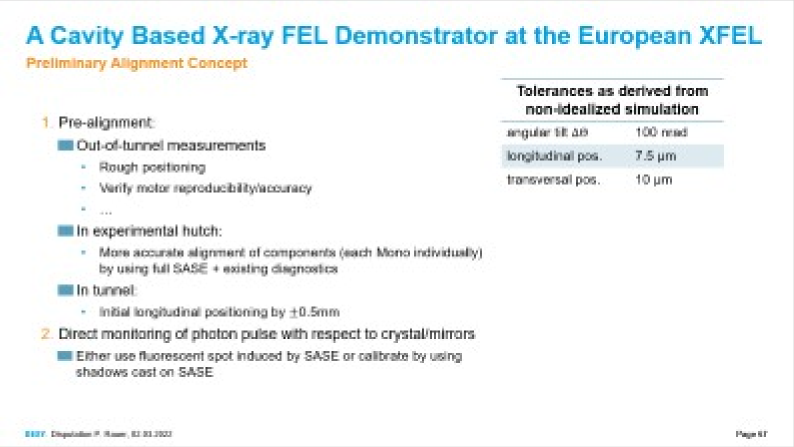
- Scheme 1: Just use the regular crystal transmission
  - Very simple → most probable scheme for initial experiment (also used for following simulations)
  - Problem of low X-ray intensity during alignment
  - Phase space of transmitted radiation is different to one of trapped radiation (next slide)



A Cavity Based X-ray FEL Demonstrator for the European XFEL

Proof of Principle Experiment: Two Compatible Transmission Schemes

- Scheme 1: Use a grating for outcoupling
  - Direct access to radiation inside the cavity (longitudinal and transverse)
  - Possibility to couple in SASE for alignment
  - More complex component-wise



A Cavity Based X-ray FEL Demonstrator at the European XFEL

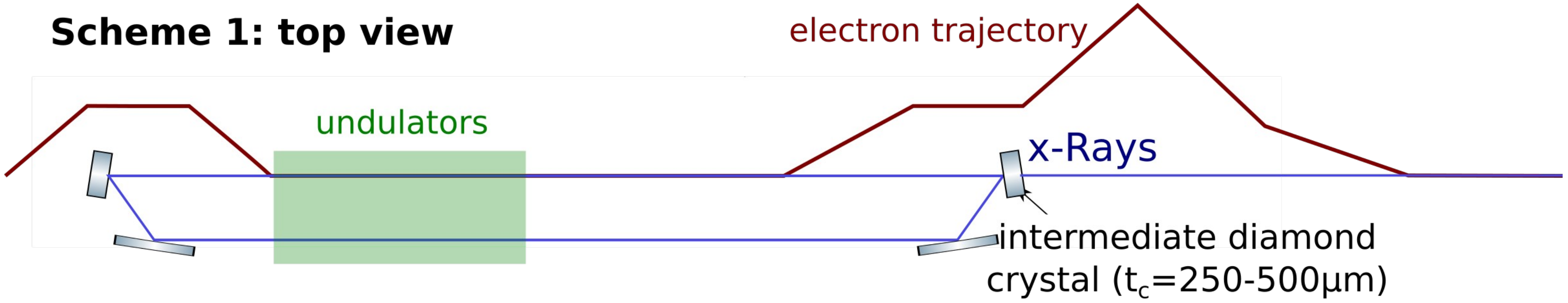
Preliminary Alignment Concept

1. Pre-alignment:
   - Out-of-tunnel measurements
     - Rough positioning
     - Verify motor reproducibility/accuracy
     - …
   - In experimental hutch:
     - More accurate alignment of components (each Mono individually) by using full SASE + existing diagnostics
   - In tunnel:
     - Initial longitudinal positioning by ±0.5mm
2. Direct monitoring of photon pulse with respect to crystal/mirrors
   - Either use fluorescent spot induced by SASE or calibrate by using shadows cast on SASE

Tolerances as derived from non-idealized simulation	
angular tilt $\Delta\theta$	100 nrad
longitudinal pos.	7.5 µm
transversal pos.	10 µm

A Cavity Based X-ray FEL Demonstrator for the European XFEL

Proof of Principle Experiment: Two Compatible Transmission Schemes



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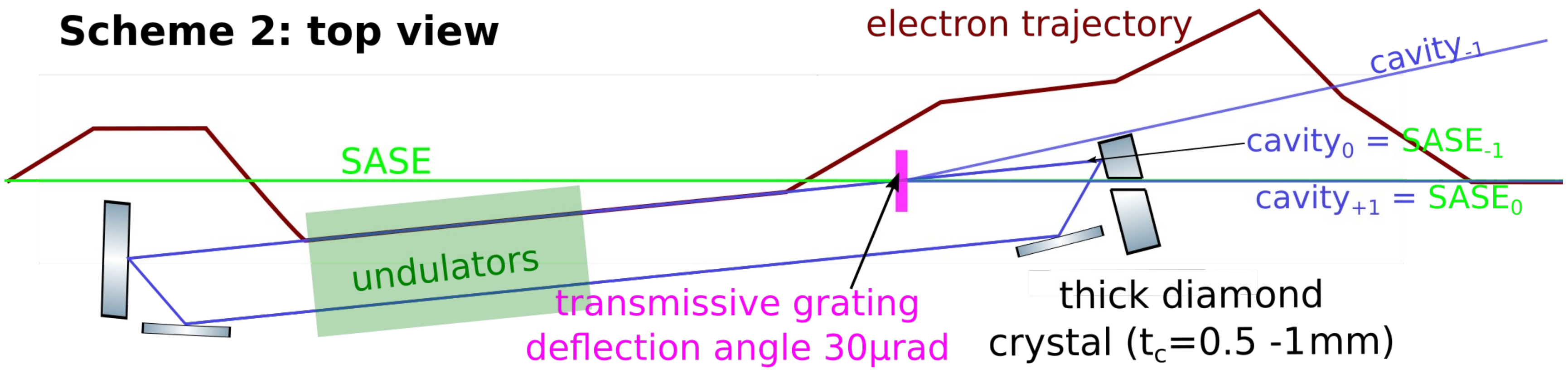
A Cavity Based X-ray FEL Demonstrator for the European XFEL

Proof of Principle Experiment: Two Compatible Transmission Schemes



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A Cavity Based X-ray FEL Demonstrator at the European XFEL

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     - Rough positioning
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     - …
   - In experimental hutch:
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2. Direct monitoring of photon pulse with respect to crystal/mirrors
   - Either use fluorescent spot induced by SASE or calibrate by using shadows cast on SASE

Tolerances as derived from non-idealized simulation	
angular tilt	100 nrad
longitudinal pos.	7.5 µm
transversal pos.	10 µm

A Cavity Based X-ray FEL Demonstrator at the European XFEL

Preliminary Alignment Concept

1. Pre-alignment:
2. Direct monitoring of photon pulse with respect to crystal/mirrors
   - Either use fluorescent spot induced by SASE or calibrate by using shadows cast on SASE
3. Fine crystal alignment (using HIREX) [in discussion if necessary]
   - Tracking the notches in transmission spectrum via angular change
   - Can reach accuracies down to 50nrad!
   - However, we need combined accuracy of Montel+crystals!

Tolerances as derived from non-idealized simulation	
angular tilt	100 nrad
longitudinal pos.	5 µm
transversal pos.	10 µm

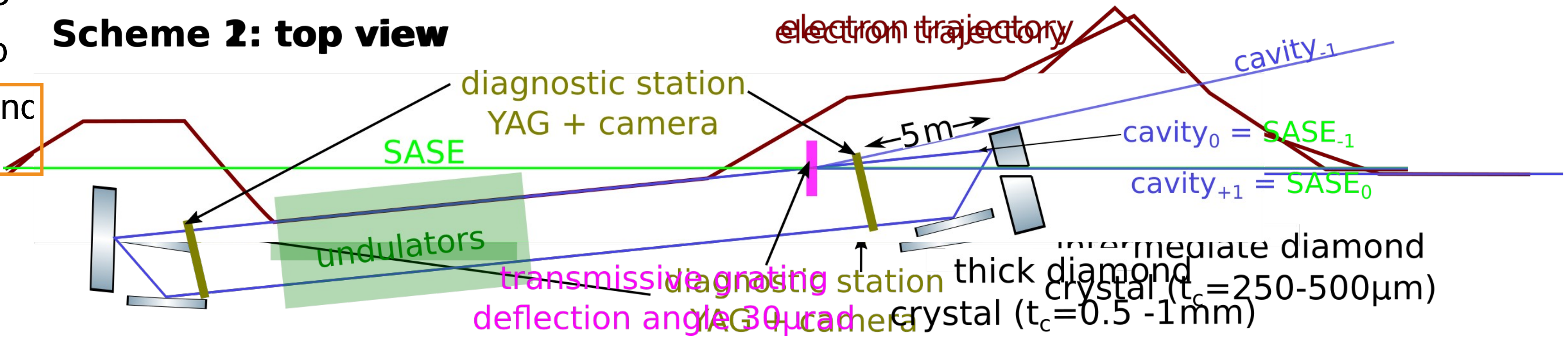
A Cavity Based X-ray FEL Demonstrator at the European XFEL

Preliminary Alignment Concept

Tolerances as derived from non-idealized simulation	
angular tilt	100 nrad
longitudinal pos.	7.5 µm
transversal pos.	10 µm

1. Pre-alignment:
2. Direct monitoring of photon pulse with respect to crystal/mirrors
3. Fine crystal alignment (using HIREX) [in discussion if necessary]
   - Tracking the notches in transmission spectrum via angular change
4. Combined alignment of mirror + crystal angle by using scintillators inside the cavity
   - First downstream Mono (also using SASE)
   - Then upstream Mono
   - Align for full roundtrip
   - Problem of backgrounc radiation

Scheme 2: top view



A Cavity Based X-ray FEL Demonstrator at the European XFEL

Preliminary Alignment Concept

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angular tilt	100 nrad
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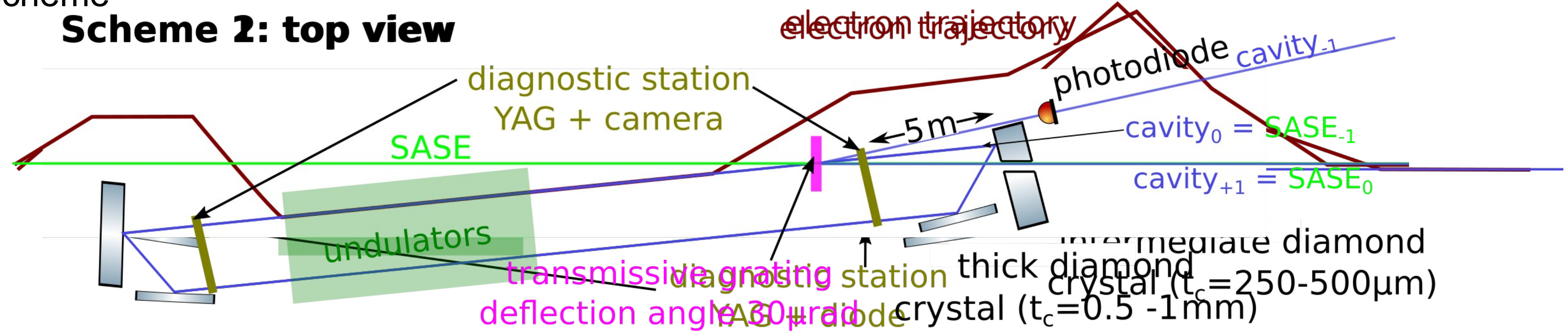
transversal pos.	10 µm

1. Pre-alignment:
2. Direct monitoring of photon pulse with respect to crystal/mirrors
3. Fine crystal alignment (using HIREX) [in discussion if necessary]
4. Combined alignment of mirror + crystal angle by using scintillators inside the cavity
5. Measure multiple round trip ring down (information on cavity losses)
    - Either use photodiodes or fast gating
    - Easier with grating scheme



A Cavity Based X-ray FEL Demonstrator at the European XFEL

Preliminary Alignment Concept

Tolerances as derived from non-idealized simulation	
angular tilt	100 nrad
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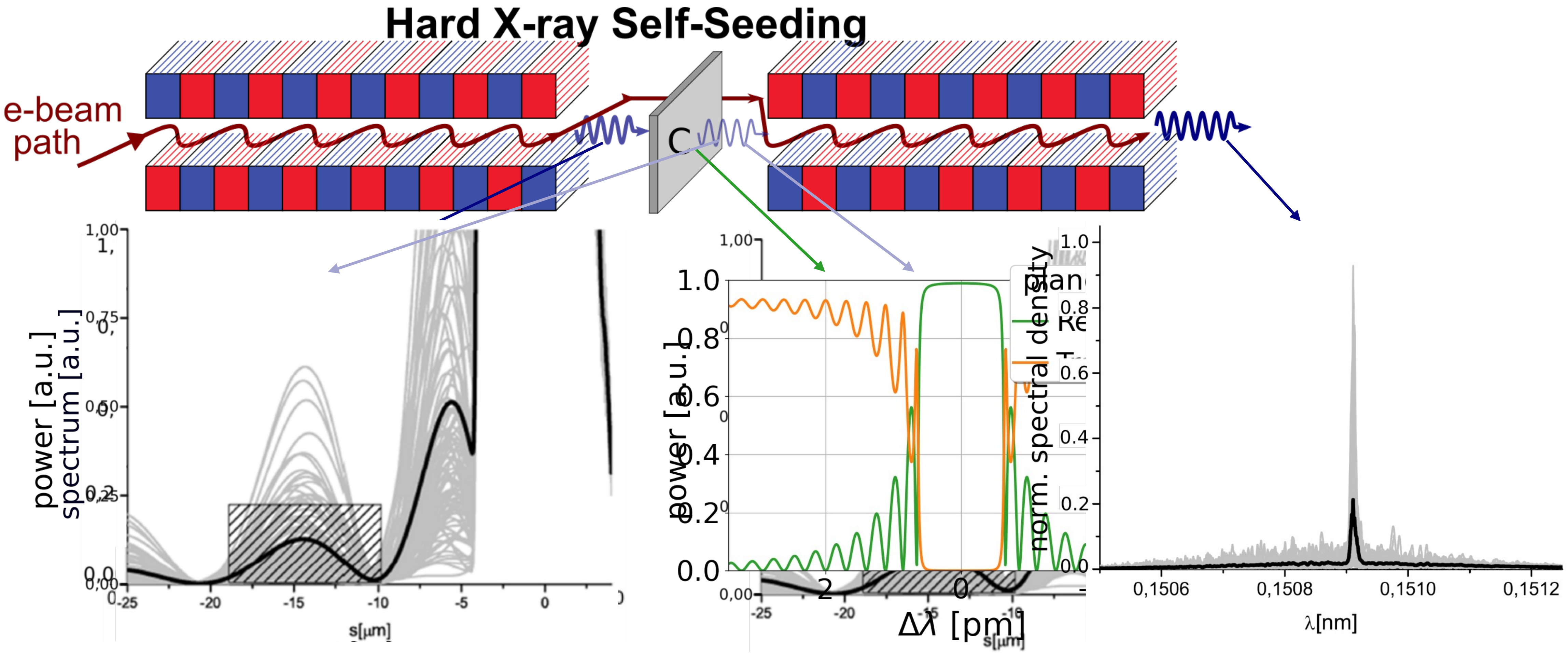
1. Pre-alignment:
2. Direct monitoring of photon pulse with respect to crystal/mirrors
3. Fine crystal alignment (using HIREX) [in discussion if necessary]
4. Combined alignment of mirror + crystal angle by using scintillators inside the cavity
5. Measure multiple round trip ring down (information on cavity losses)
    - Either use photodiodes or fast gating
    - Easier with grating scheme
6. Longitudinal alignment by looking for seeding with HIREX (in =5 µm steps)

A Cavity Based X-ray FEL Demonstrator for the European XFEL

From HXRSS to CBXFEL

🟧 *Design and Construction of Hard X-ray Self-Seeding Setups for the European XFEL*, Project Proposal, DESY, 2014



A Cavity Based X-ray FEL Demonstrator for the European XFEL

From HXRSS to CBXFEL

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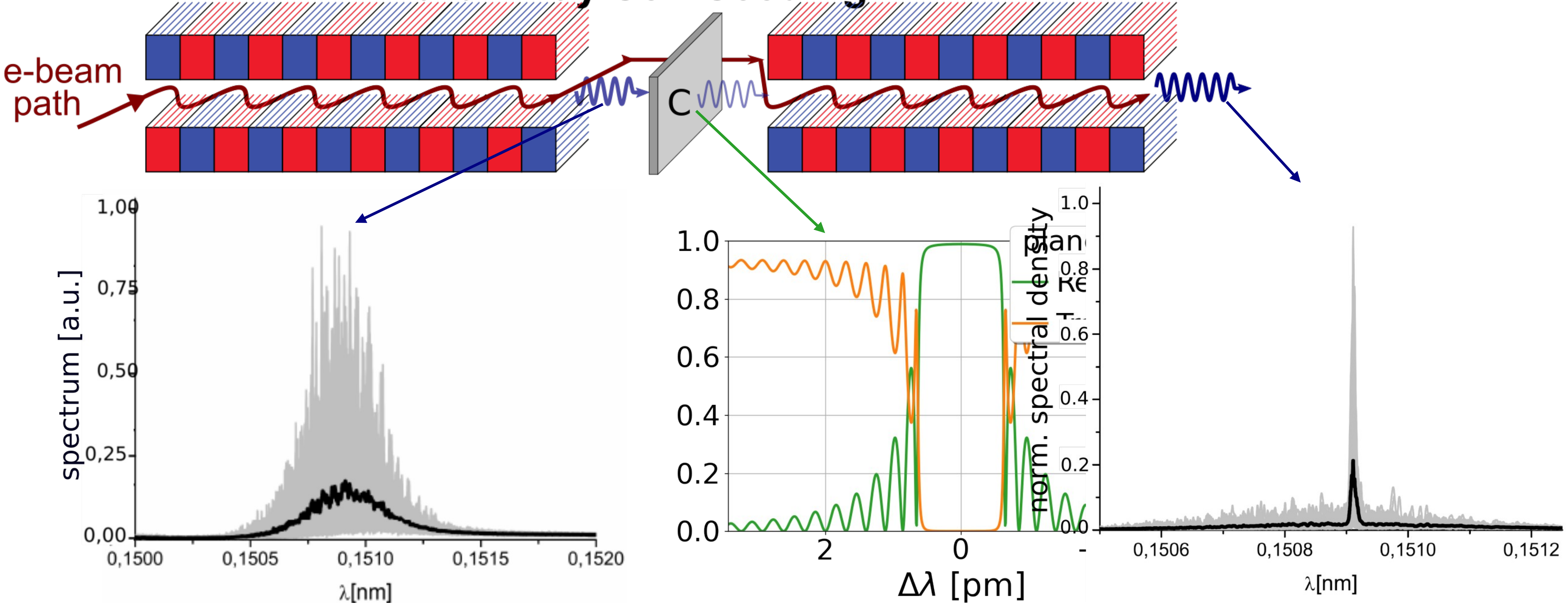
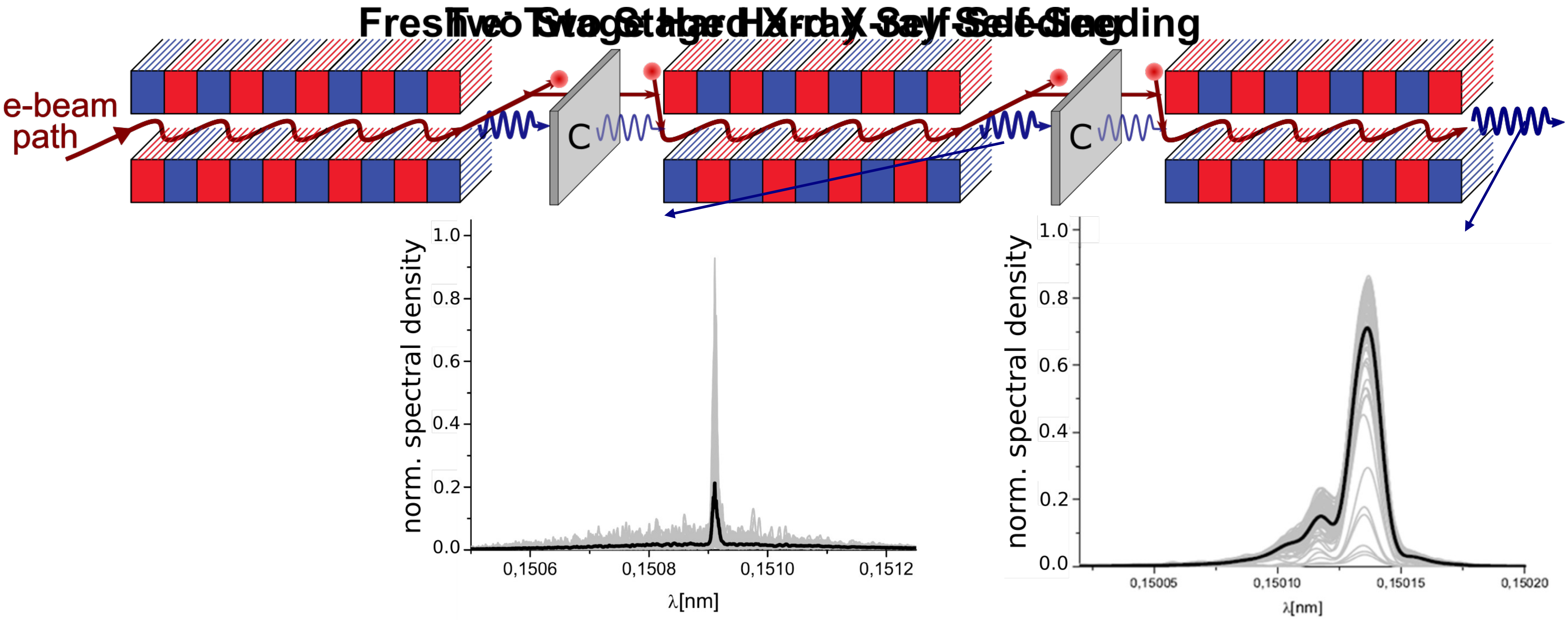
Hard X-ray Self-Seeding



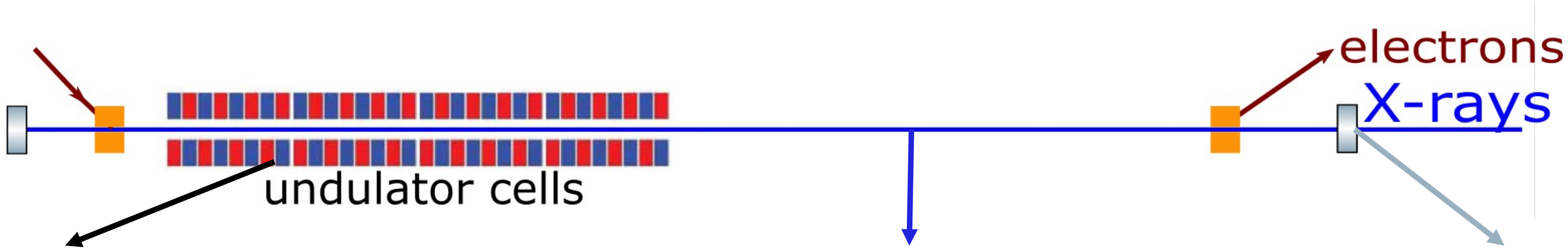
A Cavity Based X-ray FEL Demonstrator for the European XFEL

From HXRSS to CBXFEL



A Cavity Based X-ray FEL Demonstrator for the European XFEL

Start-2-End Modeling of a CBXFEL: Three Fully Coupled Submodules (+1)



FEL Process

- Using *Genesis-1.3* (V4)
  - ▶ Well known and benchmarked
  - ▶ Parallelized and fast
  - ▶ Many tunable parameters and adjustable errors

X-ray Propagation

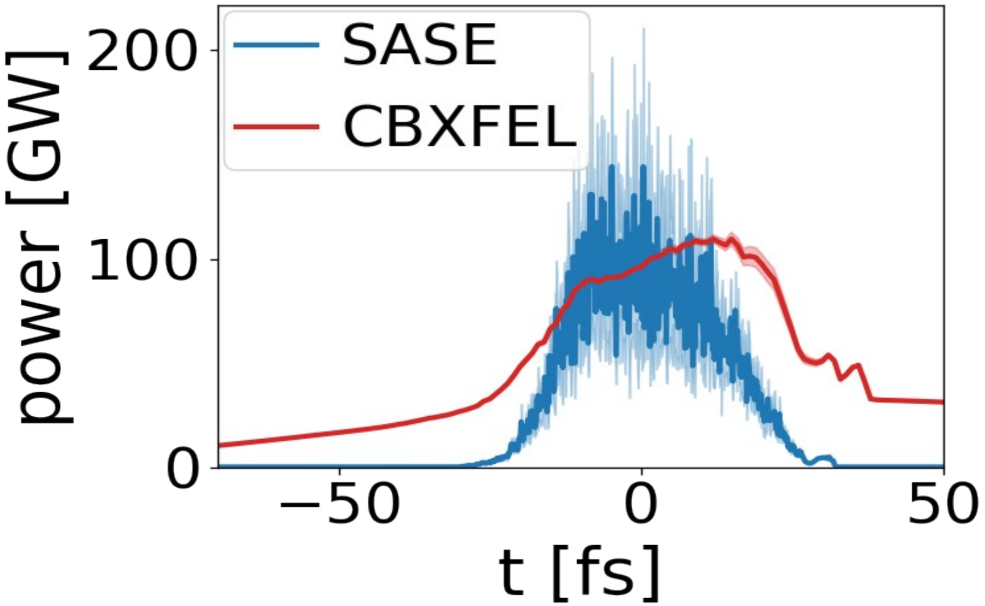
- Self-written *parallel X-ray Cavity Propagator* (pXCP)
  - ▶ Based on Fourier Optics
  - ▶ Written in C++ and making use of MPI parallelization
  - ➔ Very fast on (Maxwell) Cluster
  - ▶ Very versatile (adjustable optics and error sources)

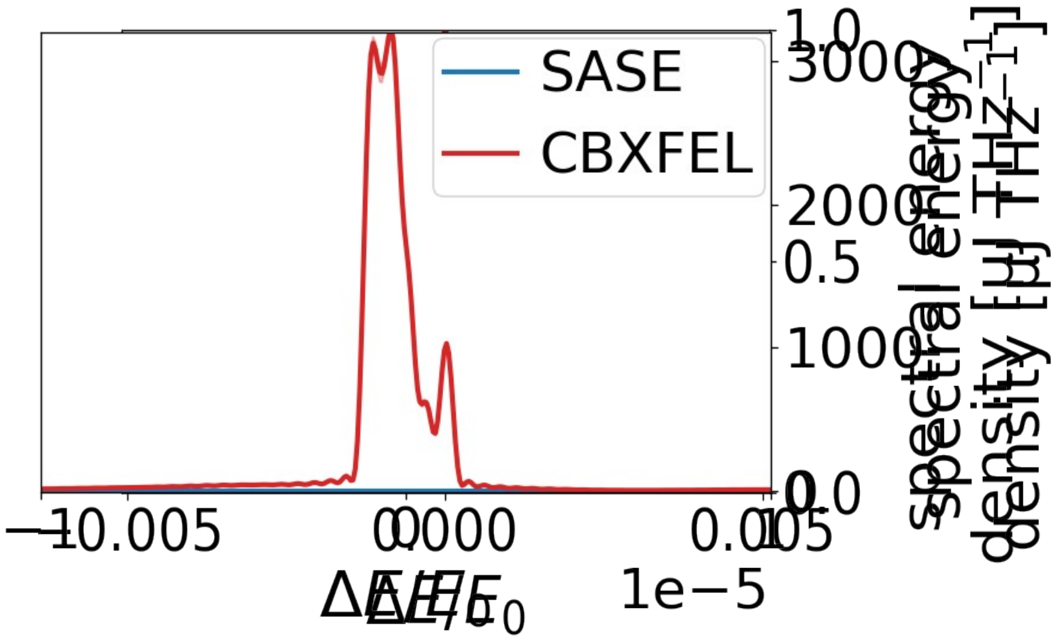
X-ray Crystal Interaction

- X-ray reflection based on (two beam) dynamic diffraction
- Crystal thermal response using COMSOL Multiphysics®
  - ▶ Based on (modified) Fourier's law of thermal conduction and quasistatic thermal expansion
  - ▶ Potentially dynamic elastic response (Thesis I. Bahns)

A Cavity Based X-ray FEL Demonstrator for the European XFEL

SASE vs CBXFEL





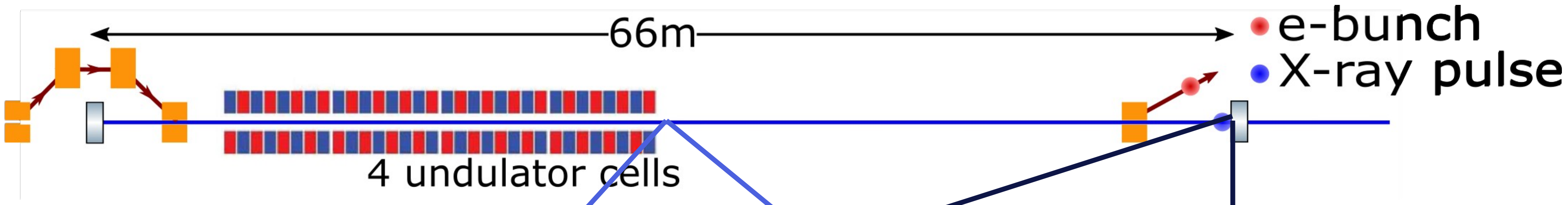
- **SASE**
  - High Powers
  - Bandwidth
  - Coherence time ~ 0.2 fs [1]
  - Pulse lengths down to ~ 1fs
  - Dependent on electron bunch

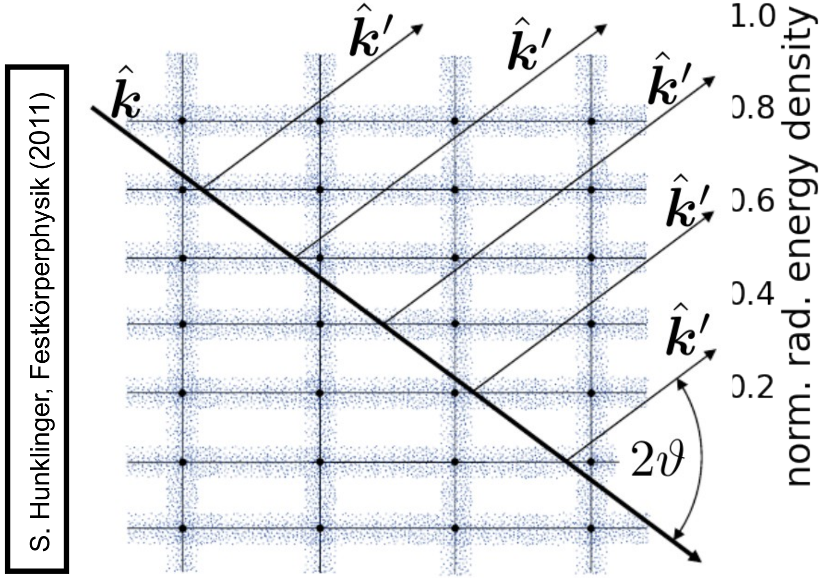
[1] G. Geloni et al., N. Jour. Phys., 12, 035021 (2010)

- **CBXFEL**
  - High Powers, potentially ~ SASE
  - Pulse lengths of ~ 100fs
  - Bandwidth
  - ~full pulse coherence (3D)
  - Dependent on crystal optics

A Cavity Based X-ray FEL Demonstrator for the European XFEL

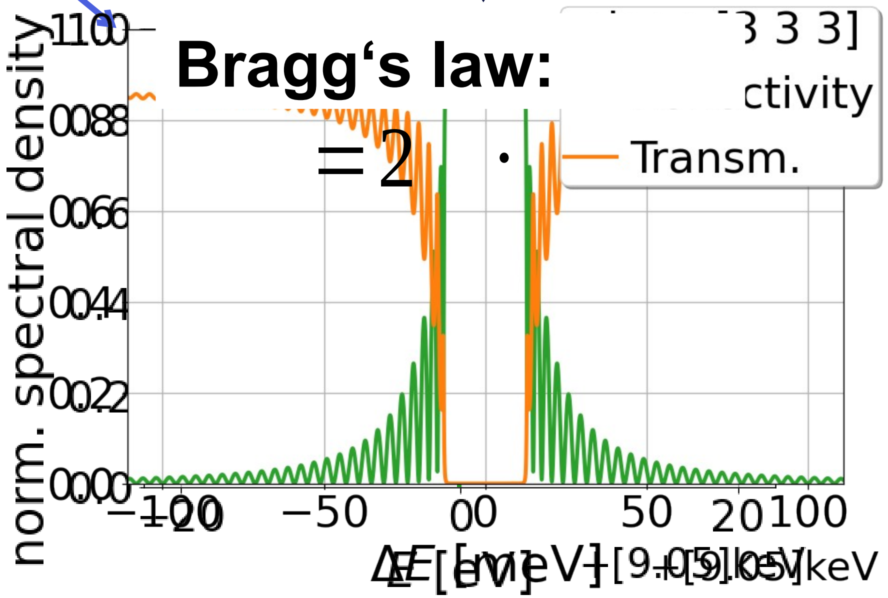
A Walkthrough





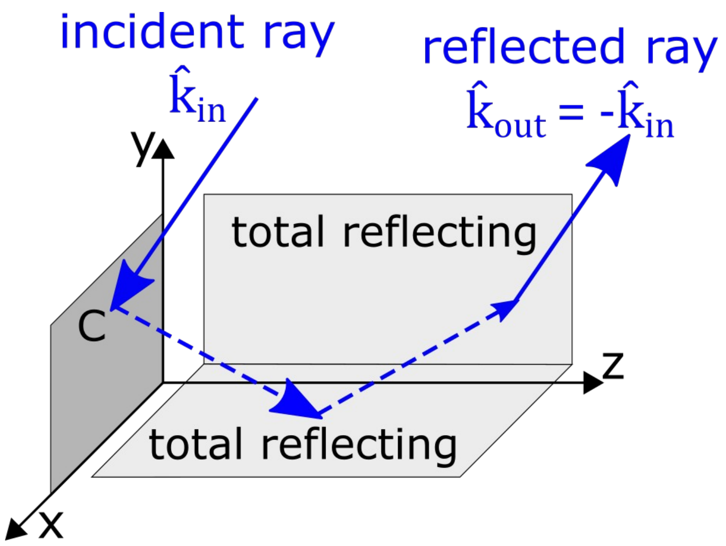
Bragg‘s law:

$= 2 \cdot$



A Cavity Based X-ray FEL Demonstrator for the European XFEL

Proof of Principle Experiment at SASE1

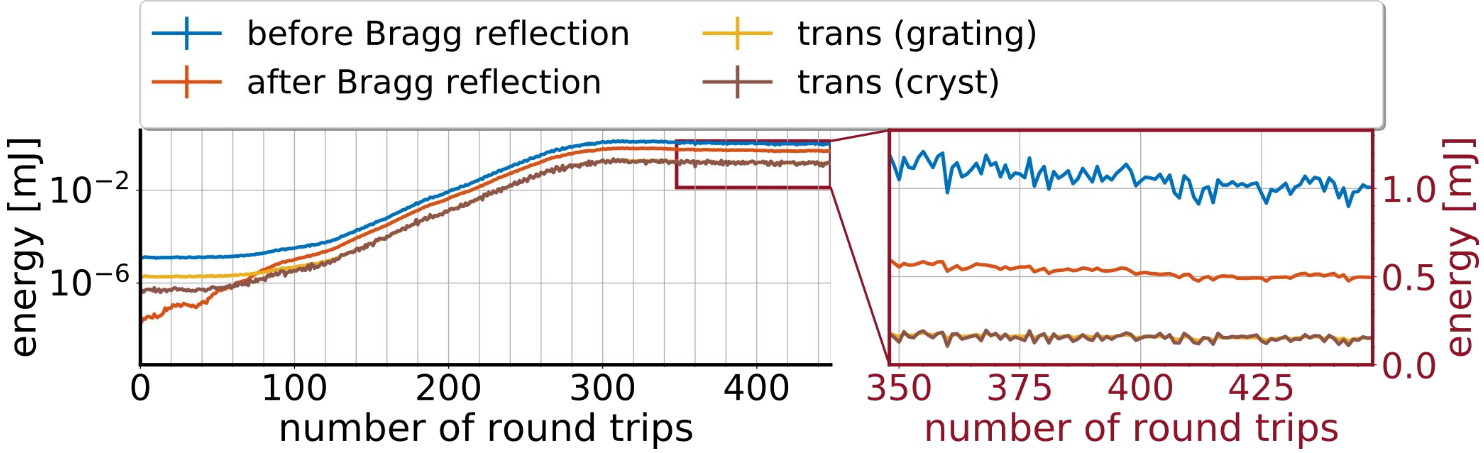


- Surface curvature to achieve focussing
- All three mirrors at 90° → Retroreflector:
  - → Decoupling from outer vibrations
- Dyadic error (not perfect 90°) → loss in compensation
  - Assuming error of 1 mrad: Still three orders of magnitude compensation!
  - 50 µrad → 100 nrad

A Cavity Based X-ray FEL Demonstrator at the European XFEL

Including Thermal Response/ Introducing additional losses/outcoupling

- Adding 15% of additional losses before downstream mirror (grating scheme)
  - Matching pulse energy in saturation to 1mJ
- Stable operation could be achieved
  - Reduced pulse energy



Simulation results	
Transmitted (grating)	
Sat. pulse energy	0.16(1) mJ
Spectral Q density	~30 µJ/THz
Brilliance	$1.9(2)*10^{33}$
Transmitted (cryst)	
Sat. pulse energy	0.15(2) mJ
Spectral Q density	~4 µJ/THz
Brilliance	$1.7(4)*10^{33}$
SASE	
Sat. pulse energy	~3 mJ
Spectral Q density	~0.5 µJ/THz
Brilliance	$\sim 5*10^{33}$

A Cavity Based X-ray FEL Demonstrator at the European XFEL

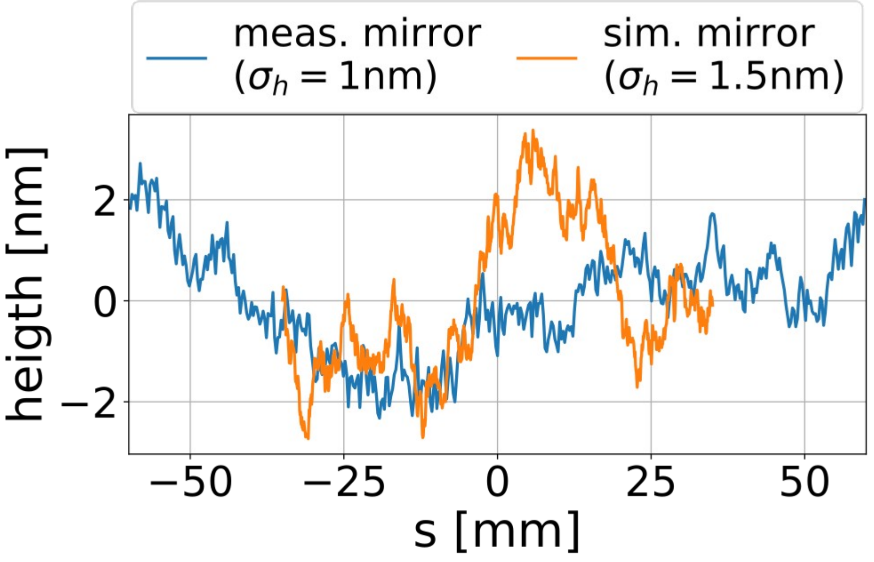
Non-Idealized Case: What (most relevant) error sources are there?

- Electron beam jitter (shot to shot fluctuations)
  - transverse position jitter (3 µm)
  - pointing jitter (100 nrad)
  - timing jitter (20 fs)
  - beam energy jitter (1.7 MeV) → **reduces stability**

quite robust!

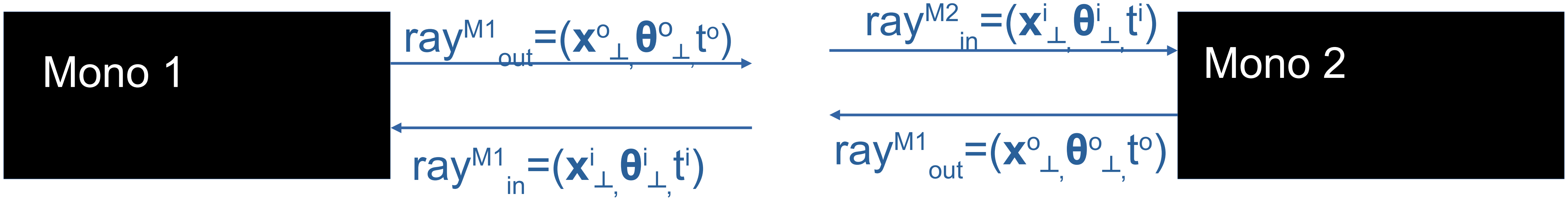
- Optical components
  - Grazing incidence mirror length: 7 cm
  - tilt of crystal: tolerance 00 nrad per crystal
  - Cavity length: tolerance 0 µm → µm
  - Mirror surface error: 1.5 nm

- W. Q. Hua et al., *Using the power spectral density method to characterize and measure the x-ray mirrors surfaces*, Proceeding of 4th IPAC, (2013)



XFELO-project: Alignment Concept

Monochromators: Relevant Degrees of Freedom



Mono 1

$\text{ray}^{M1}_{out}=(\mathbf{x}^{o}_{\perp},\boldsymbol{\theta}^{o}_{\perp},t^{o})$

$\text{ray}^{M1}_{in}=(\mathbf{x}^{i}_{\perp},\boldsymbol{\theta}^{i}_{\perp},t^{i})$

$\text{ray}^{M2}_{in}=(\mathbf{x}^{i}_{\perp},\boldsymbol{\theta}^{i}_{\perp},t^{i})$

$\text{ray}^{M1}_{out}=(\mathbf{x}^{o}_{\perp},\boldsymbol{\theta}^{o}_{\perp},t^{o})$

Mono 2

- Action of Mono 1 + Mono 2:
  - $\text{ray}^{M1}_{out} = \text{ray}^{M2}_{in} + (\Delta\mathbf{x}_{\perp},\Delta\boldsymbol{\theta}_{\perp},\Delta t)$

$\Delta\mathbf{x}_{\perp}$ [µm]	$\Delta\boldsymbol{\theta}_{\perp}$ [nrad]	Δt [µm]
10	200	10

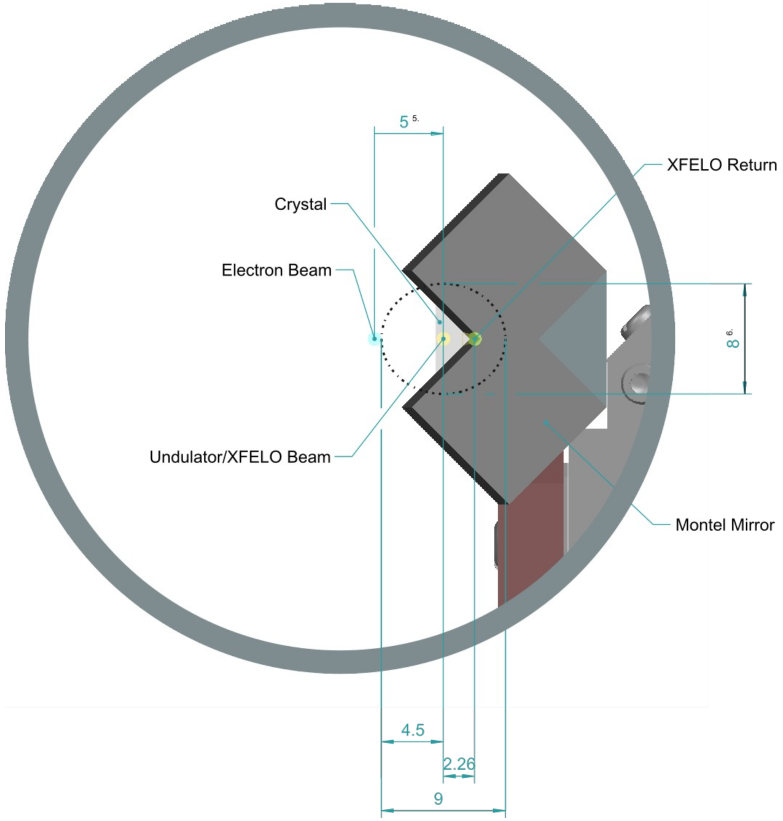
- Joint tuning: 7D phase space (without individual Mono components) ← infeasible!
- Tune every Mono on its own!

XFELO-project: Alignment Concept

Monochromators: Inside the black box

Mono 2

Retro-reflecting Monochromator2
(view from upstream to downstream)



Mirror frame (nominal):

$$\hat{\ }_1=\begin{pmatrix} (\ \ ) \\ (\ \ ) \\ 0 \end{pmatrix}, \hat{\ }_2=\begin{pmatrix} -\ \ (\ \ ) \\ (\ \ ) \\ 0 \end{pmatrix}, \hat{\ } =\begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}$$

- Some (nominal) parameter
  - Position crystal/X-ray intersection: (x,y)=(0,0)
  - Distance center KB1 to crystal: $l_{C\text{-}KB1}$= 255mm
  - Angle of incidence on KBs: θ_{In}= 3.1mrad
  - Yaw of Kbs: α=-π/4

$\left.\begin{matrix} \\ \\ \end{matrix}\right\}$

- (Roll,Pitch) = (4.4 mrad, 0)
- $(x,y)_{out}$ = $2*(\text{Roll, Pitch})_C*l_{C\text{-}KB1}$= (2.26mm, 0)