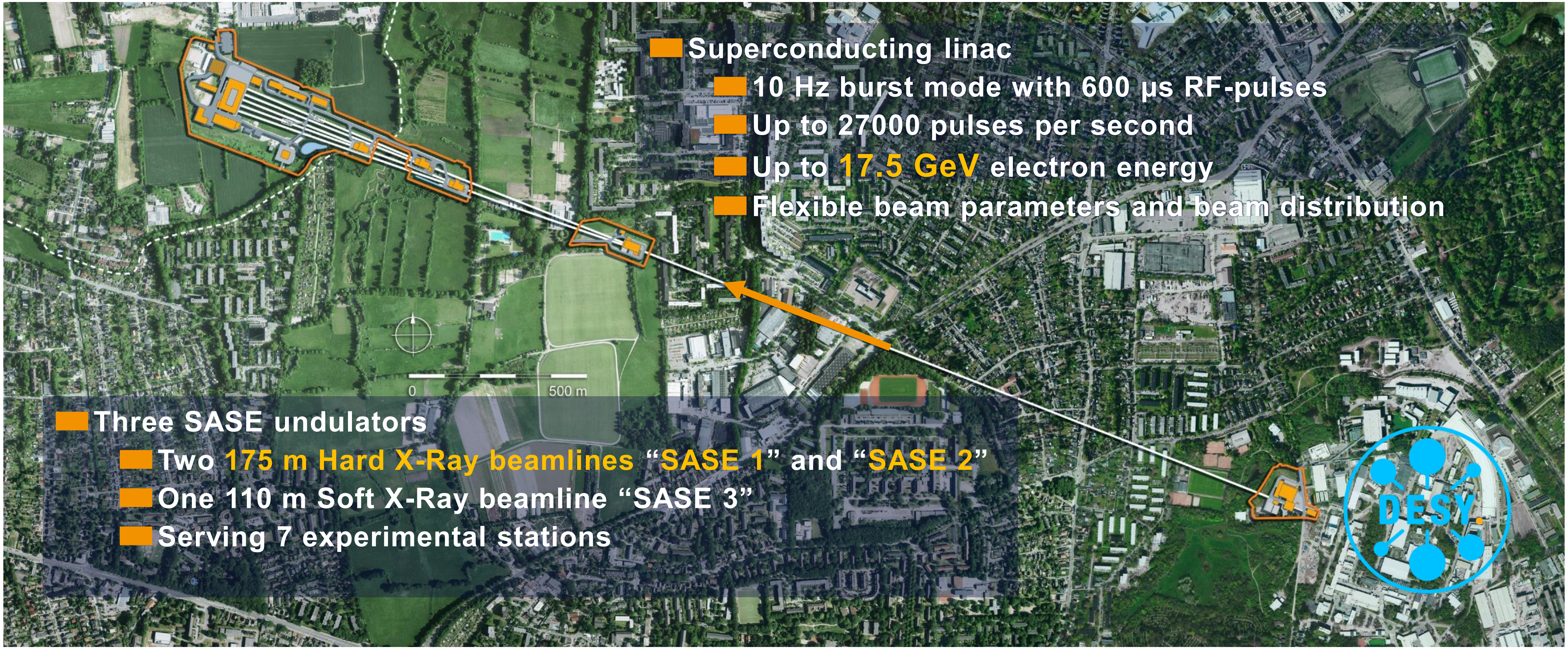
Towards Sub-Ångström Working Regime of the European X-Ray Free-Electron Laser: Simulations and First Experimental Results

Frank Brinker for the EuXFEL and DESY Team

IPAC at Venice, May 9th 2023

European XFEL

from Hamburg to Schleswig-Holstein



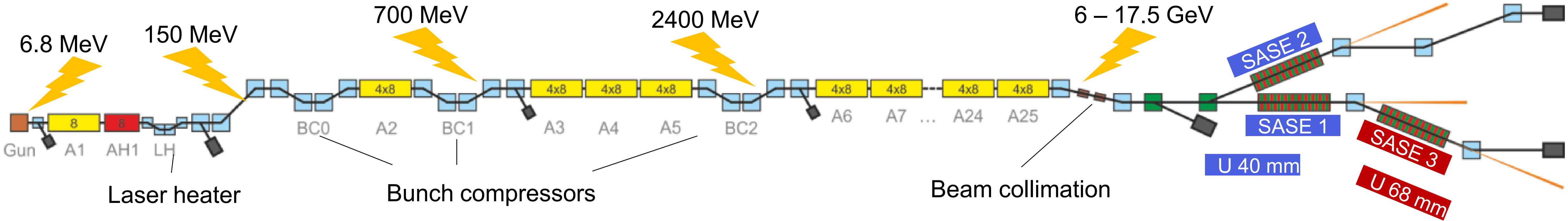
- Superconducting linac
  - 10 Hz burst mode with 600 μs RF-pulses
  - Up to 27000 pulses per second
  - Up to 17.5 GeV electron energy
  - Flexible beam parameters and beam distribution

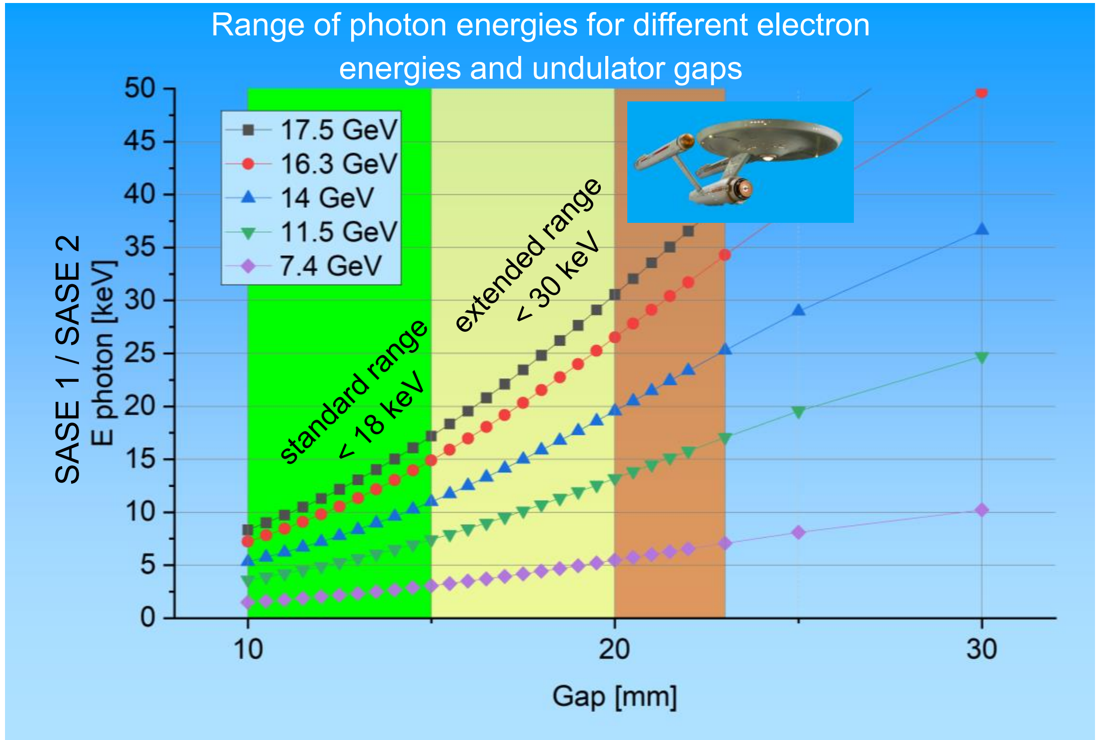
- Three SASE undulators
  - Two 175 m Hard X-Ray beamlines “SASE 1” and “SASE 2”
  - One 110 m Soft X-Ray beamline “SASE 3”
  - Serving 7 experimental stations

Content

- Standard wavelength range of the EuXFEL
- Scientific case for higher photon energies
- Going for 24 / 30 keV
  - Simulations
  - Experimental results at 24 and 30 keV, Run 1
  - SASE 2 Run 2, photon transport
  - Problems in Run 2
- Future developments
  - Improved beam properties
  - After burner, SC undulators
  - Harmonic lasing

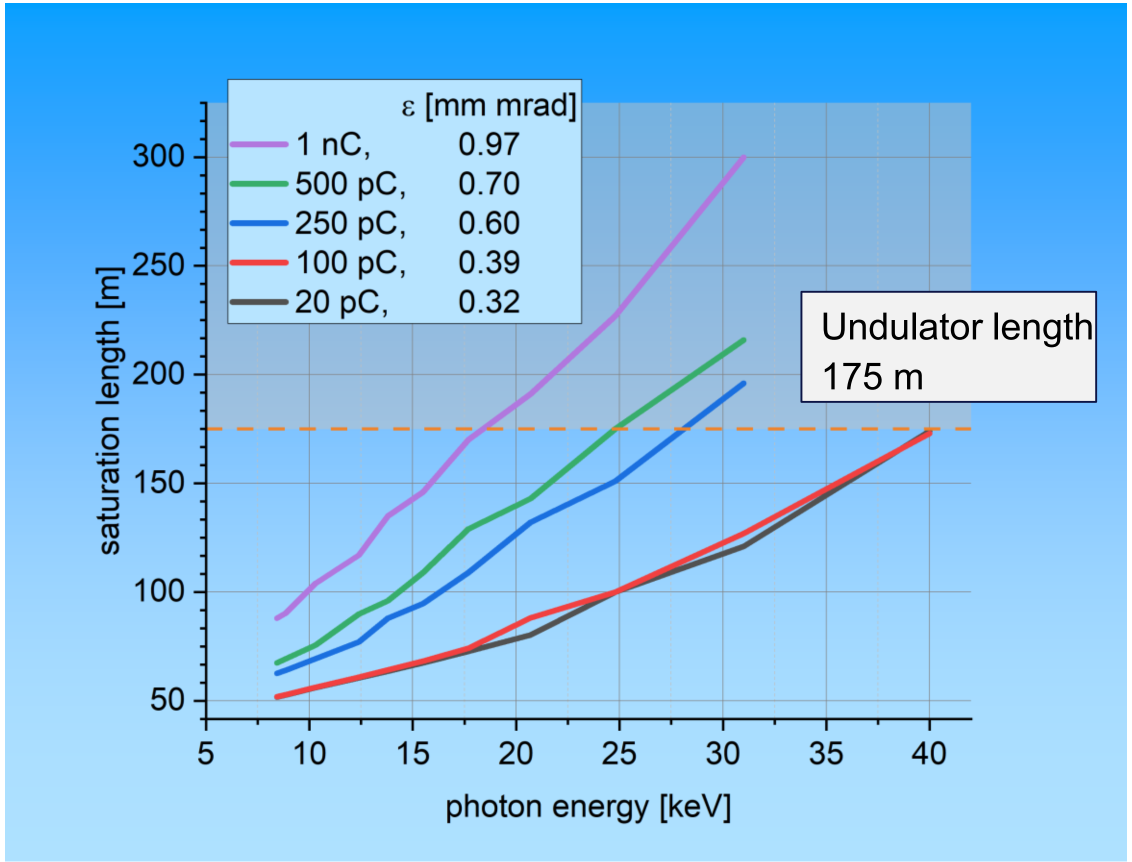
Facility overview



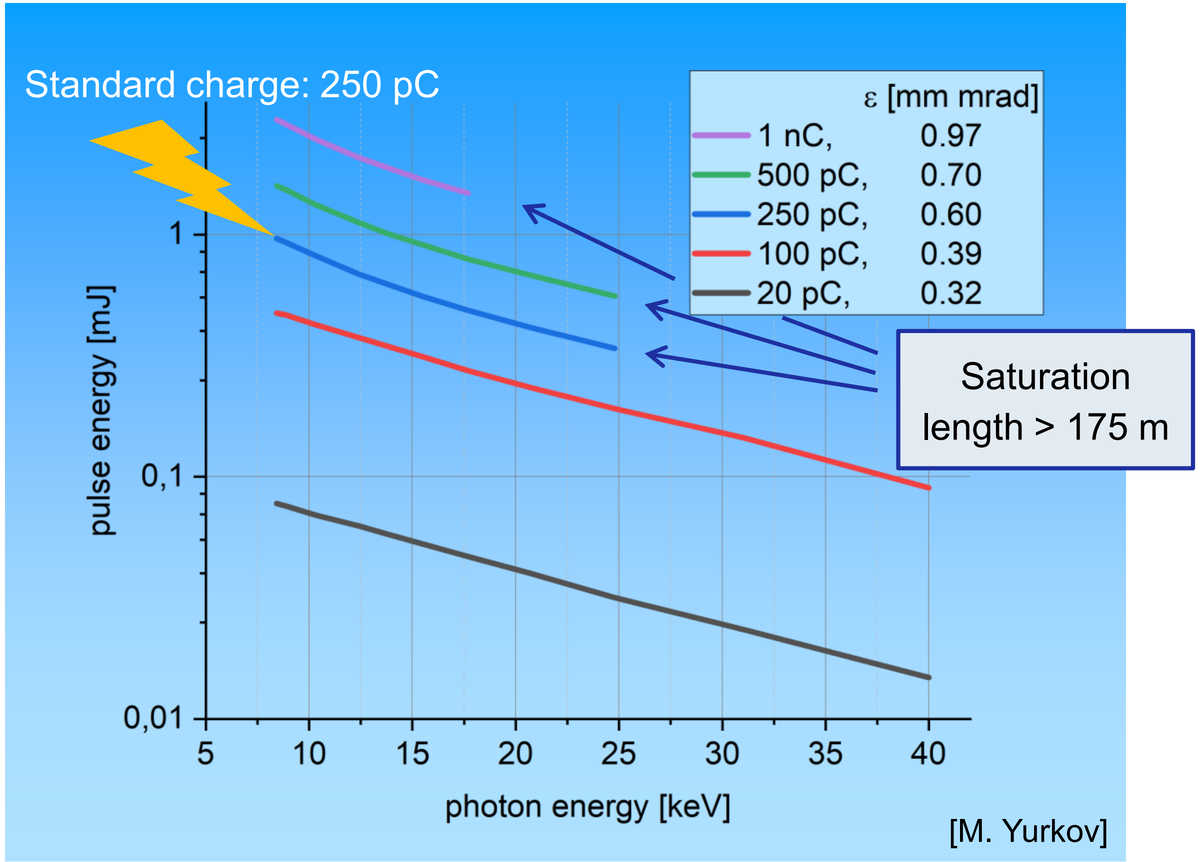


- Standard operation presently covers the range up to 18 keV
  - Gap < 15 mm, K > 2.5
  - Sase setup is straightforward with shorter gain length
  - Intensities higher
- Up to 30 keV could be reached in test runs
- To reach significant intensities beyond that, new schemes have to be explored

What performance can we expect at high energies with 17.5 GeV for different emittances/charges?



Undulator length 175 m



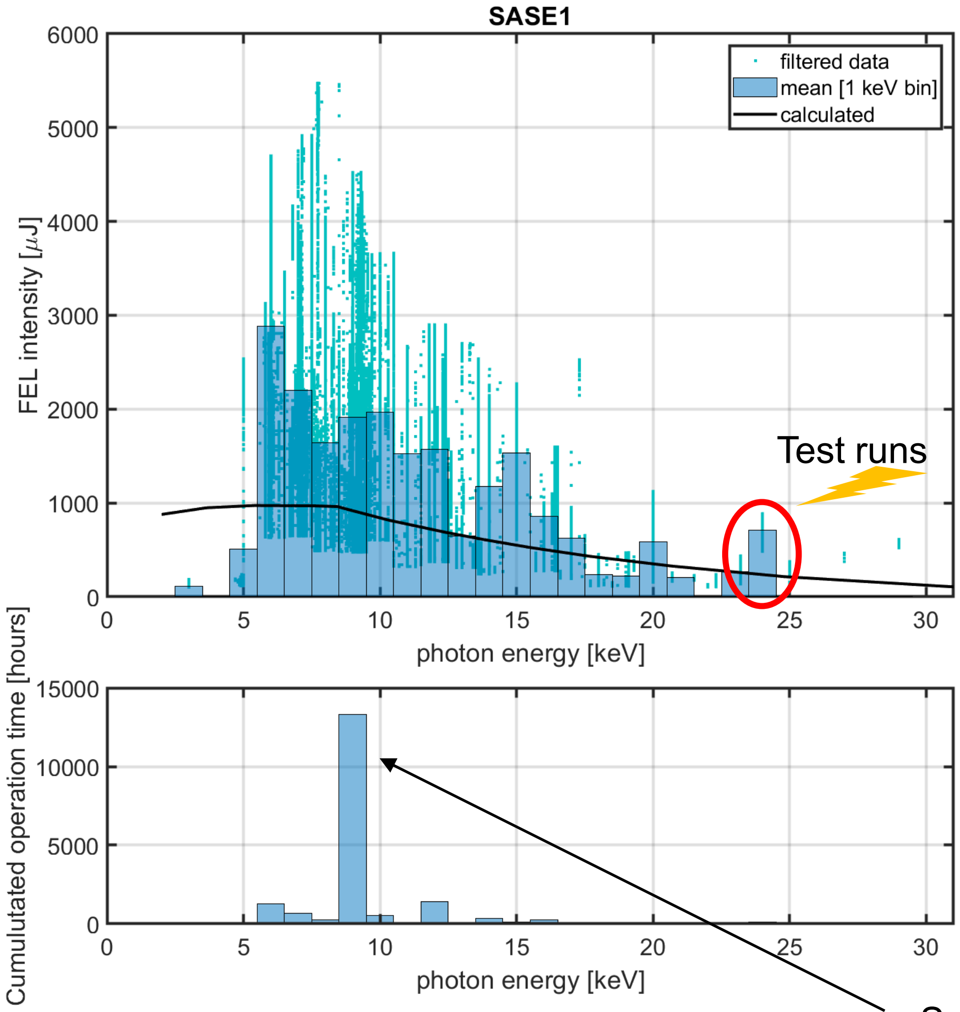
Standard charge: 250 pC

Saturation length > 175 m

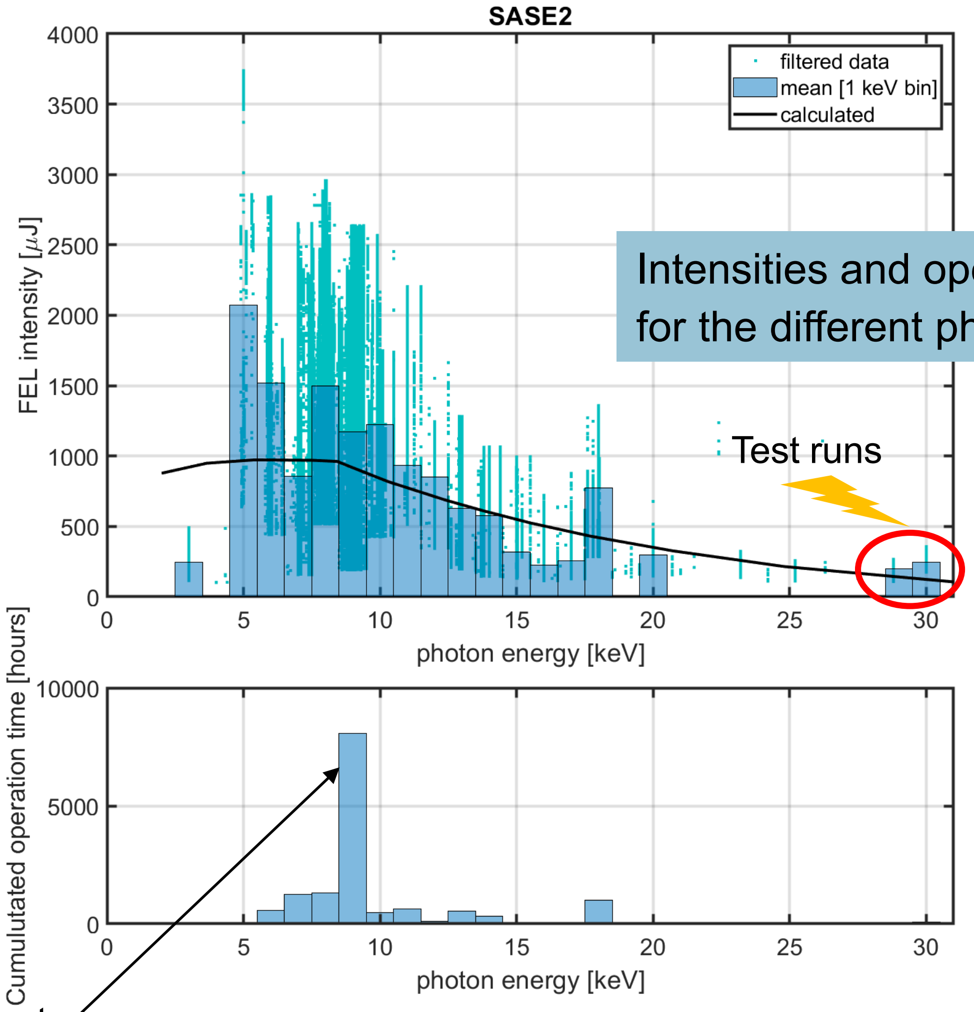
[M. Yurkov]

SASE calculations with “FAST” until **point of saturation** using a bunch with moderate emittance and energy spread. **With post saturation taper significantly higher values can be reached**.

Requested photon energies and intensities reached during the last years



Test runs

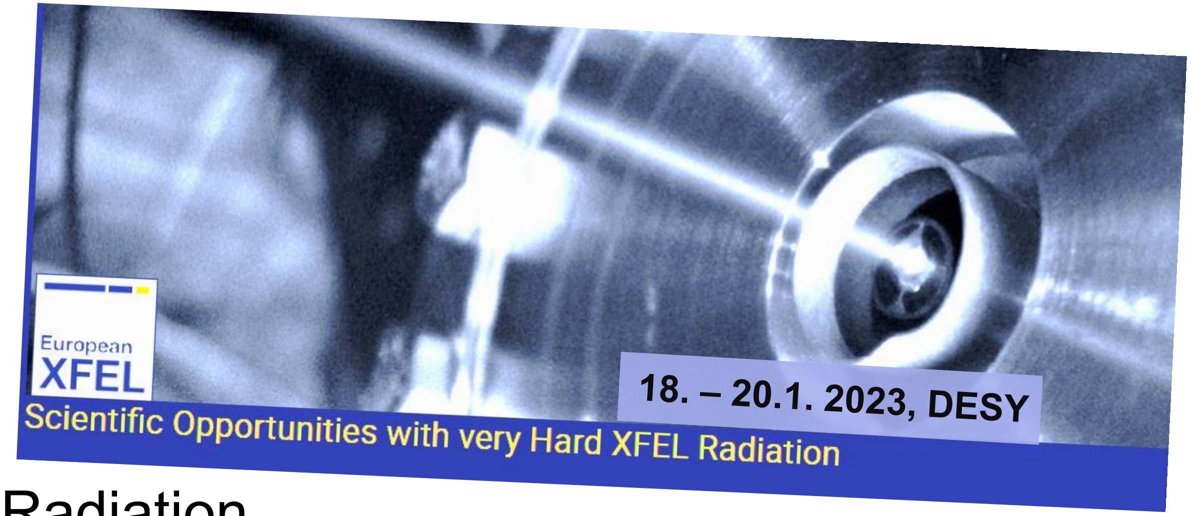


Test runs

Intensities and operation times for the different photon energies

Just last week:
Runs with 19 keV
and 23 keV

Sweep spot
9 keV



Is there a need for shorter wavelengths?

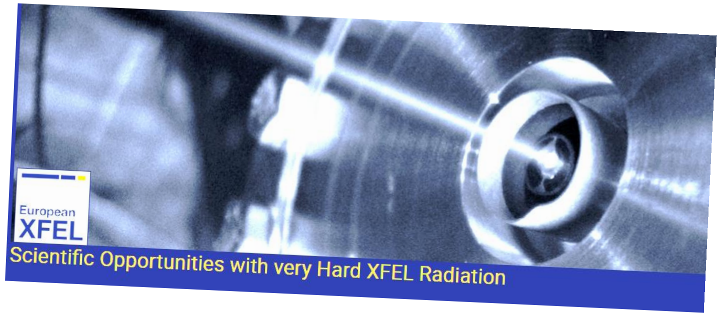
EuXFEL Workshop in HH, January 23’:

Scientific Opportunities with very Hard XFEL Radiation

Sessions:

- Applied Materials and Industrial Applications
- Structural Dynamics in Disordered Materials
- Dynamics of Functional Materials
- Enabling Techniques and Instrumentation for New Scientific Avenues
- High Pressure, Planetary Science and Geology, Electron Dynamics, Warm Dense Matter, Relativistic Laser Plasma, Strong Field Science

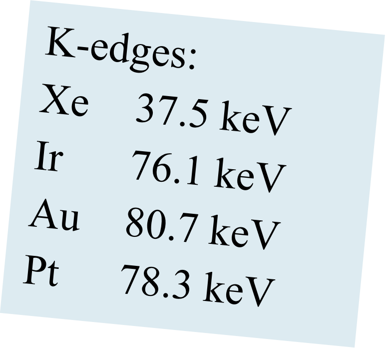
The Scientific Case for high photon energies



Scientific Opportunities with very Hard XFEL Radiation

Major advantages coming up for all applications:

- **High Q-range coverage**: Larger momentum transfer at moderate scattering angles (> 40 keV)
- **High penetration**: Larger penetration depth for bulk sensitivity
- **Access to K-edge spectroscopy of high-Z materials**: Enabling tracking of chemical dynamics for high-Z materials and for high-Z materials under extreme (hot, high pressure) conditions.



K-edges:

Xe	37.5 keV
Ir	76.1 keV
Au	80.7 keV
Pt	78.3 keV

The specific advantages of FELs compared to storage ring sources:

- Higher **brightness** – small **bandwidth**
- **Large transvers and longitudinal coherence**: Better contrast, phase measurements
- **Very short pulses (~fs)**: single shot imaging, freezing of dynamic processes (dynamic laser compression, ultra cold liquids, …)
- **variable pump-probe delay** from few fs to ms

See also the talk today about „Hard X-Ray self seeding“,

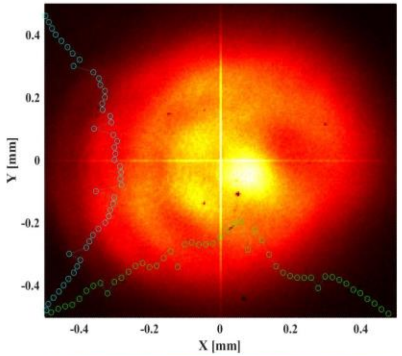
Going for 24 / 30 keV

Tracking through the linac

Collective effects included in the simulations:

- 3D space-charge
- wake fields
- CSR effects

[Y. Chen, et.al.]

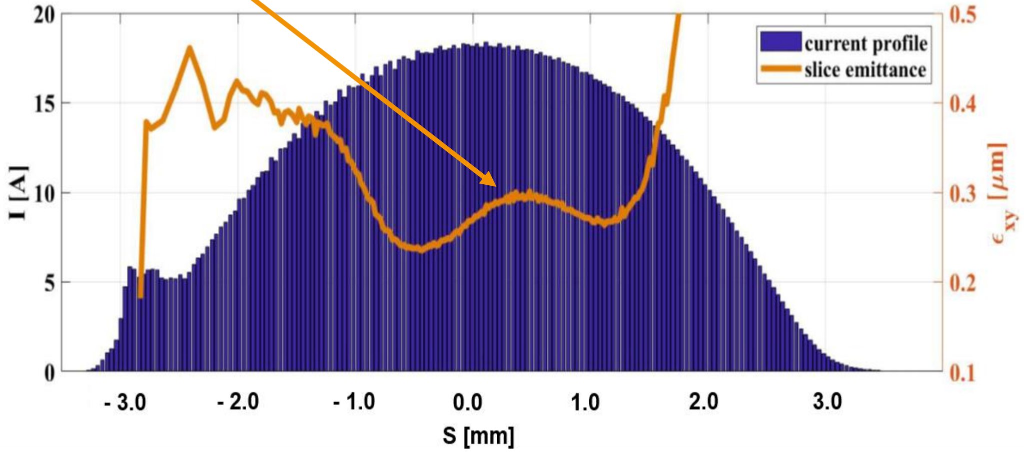


Starting with the laser

Reconstruction of the **measured transverse laser profile** as used in the simulation studies.

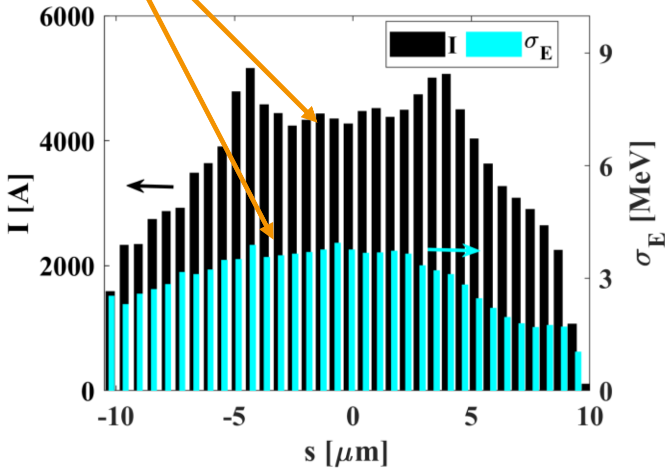
Bunch qualities after the injector and 16.3 GeV in front of the undulator beamline SASE1.

- ~0.3 mm mrad injector emittance



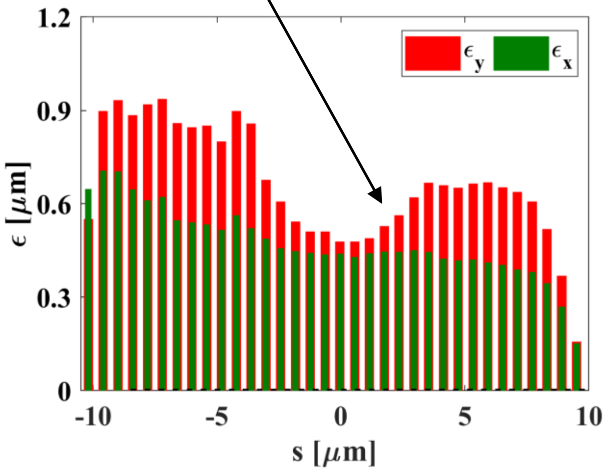
Optimized bunch current distribution (left axis) and slice emittance (right axis) along the bunch at the injector exit.

- 4.5 kA peak current
- 3.5 MeV energy spread



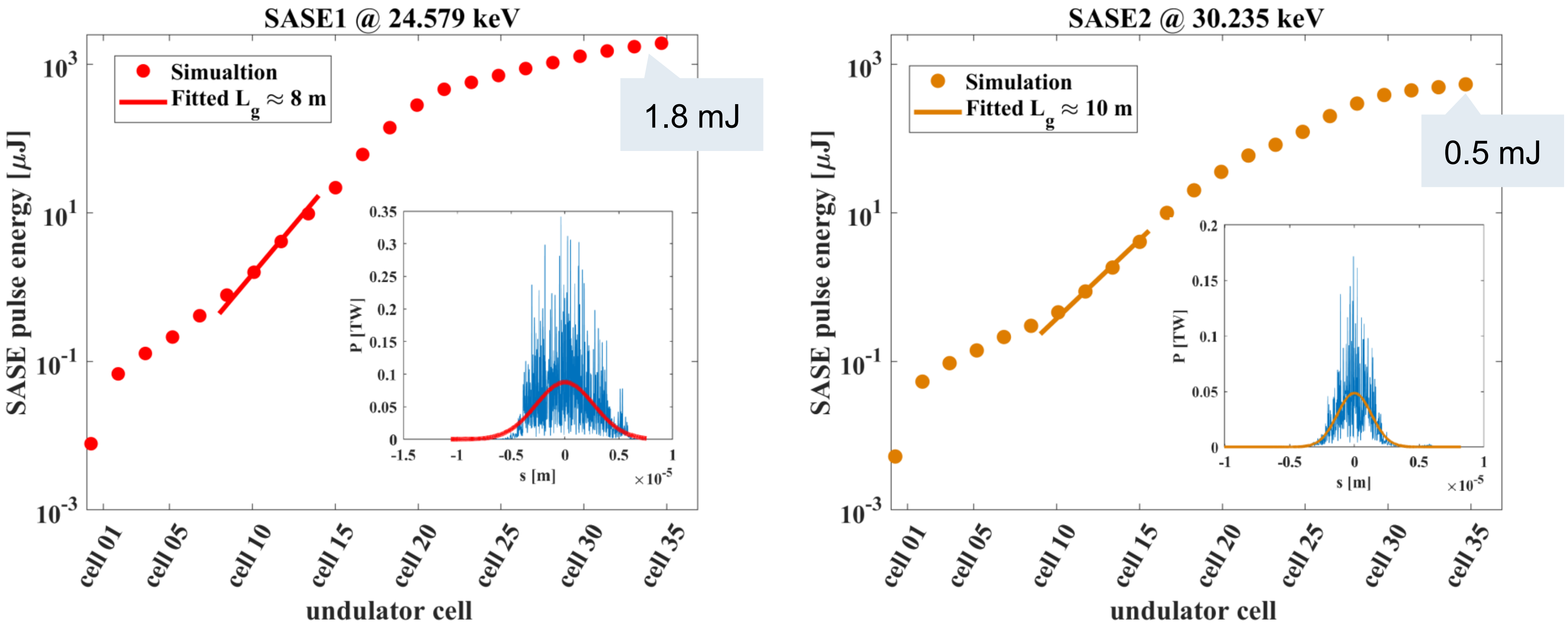
Peak current (left axis) and slice energy spread (right axis)

- ~0.6 mm mrad emittance



Slice horizontal (green) and vertical (red) emittance.

Optimized SASE performance for SASE1 (24 keV) and SASE2 (30 keV)



1.8 mJ

0.5 mJ

Simulation

Simulated SASE intensities at 24.58 keV (left) and 30.24 keV (right) for beamlines SASE1 and SASE2, respectively. The linear and quadratic taper is optimized, no alignment errors! [Y. Chen]

Going the step to the real machine:
1st try: October 2021

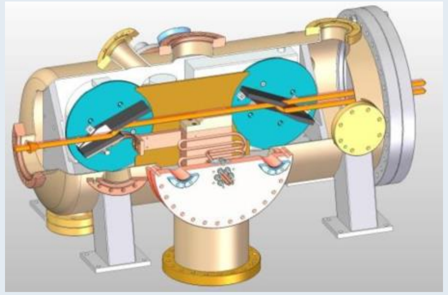
- *We started from an already good machine setup*
  - recent beam based alignment of quadrupoles in the undulator section
  - emittance optimization
  - dispersion correction

- *Therefore we could begin right away with optimizing the beamlines*
  - Increase the energy stepwise → keep enough signal for tuning
  - Optimization of
    - ► the trajectory with correctors (few µm level)
    - ► Phase between undulators with phase shifters
    - ► Pointing of individual undulators using the “K-Mono”
    - ► Linear and quadratic taper of the undulators

That’s the hard work

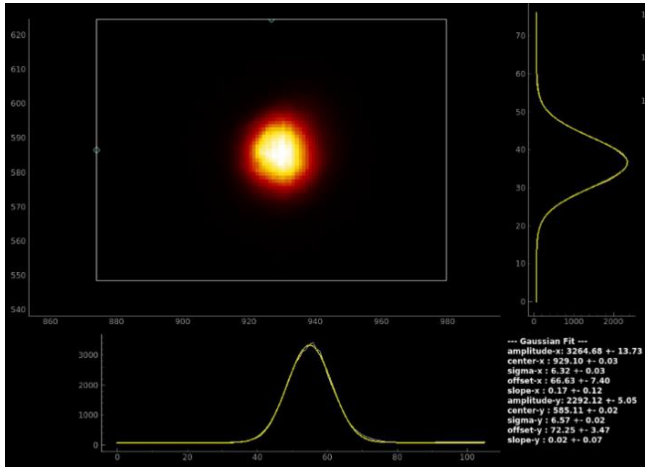
K-Mono alignment of the first 7 cells at SASE 2

K-Mono: Monochromator to analyze the pointing and wavelength of the spontaneous radiation from a **single undulator**.



[W. Freund]

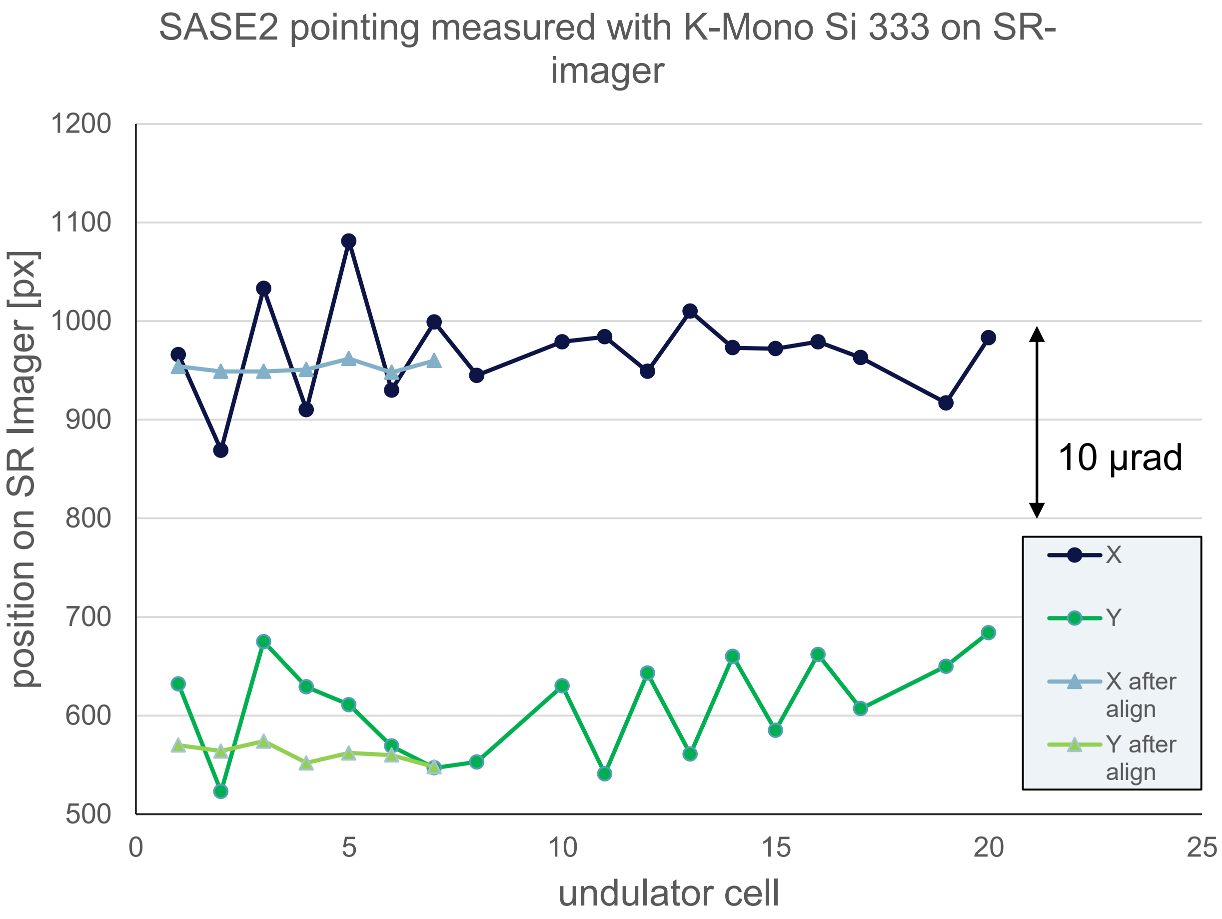
- The precision of the bba suffers at the beginning and the end of the beamline from less BPMs
- The K-Monochromator helps to overcome this by showing the pointing of individual undulators
- It also gives an absolute energy calibration



```
--- Gaussian Fit ---
amplitude-x: 3264.68 +- 13.73
center-x : 929.10 +- 0.03
sigma-x : 6.32 +- 0.03
offset-x : 66.63 +- 7.40
slope-x : 0.17 +- 0.12
amplitude-y: 2292.12 +- 5.05
center-y : 585.11 +- 0.02
sigma-y : 6.57 +- 0.02
offset-y : 72.25 +- 3.47
slope-y : 0.02 +- 0.07
```

Example image from the K-Mono after SASE 2 measured energy: 30.57 keV

Si(333)

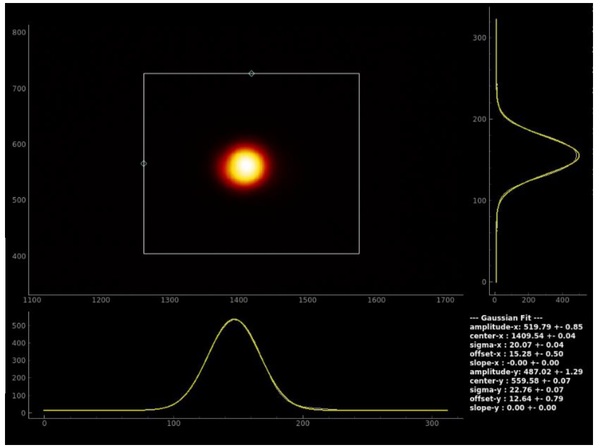


Tuning Summary SASE1, 24keV, Oct. 2021

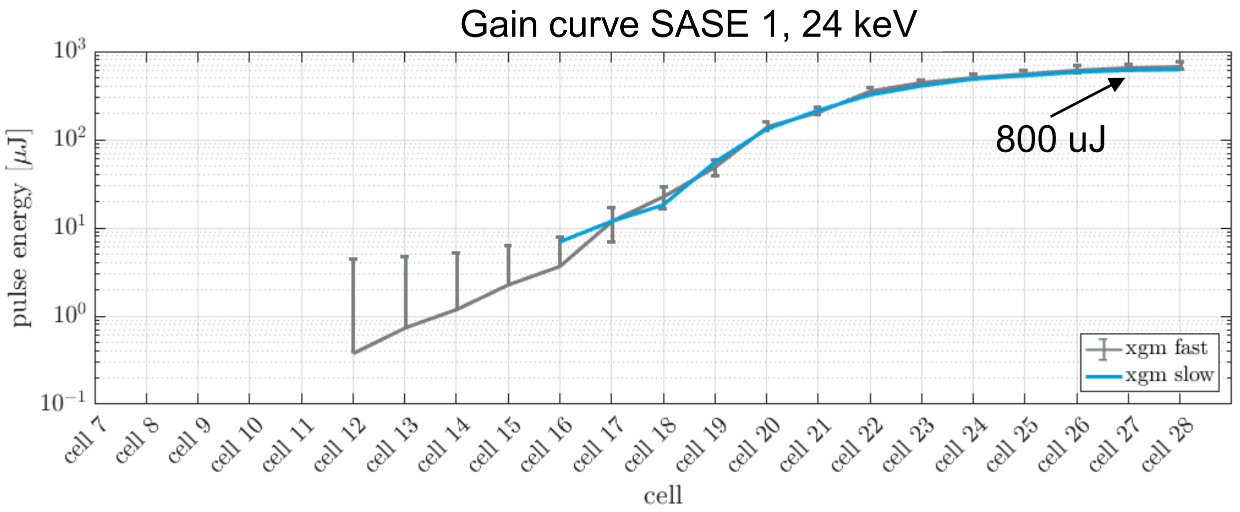
- Stepwise increase of the photon energy while maintaining some intensity allowed further optimization during the following days.
- The last 7-9 cells did not contribute first
- The adjustment of the pointing of the individual undulators (K-Mono) did help for another 2-3 cells – this method is promising but needs further improvement
- At the end the intensity was about **800 uJ** which is not so far from the maximum what could be expected

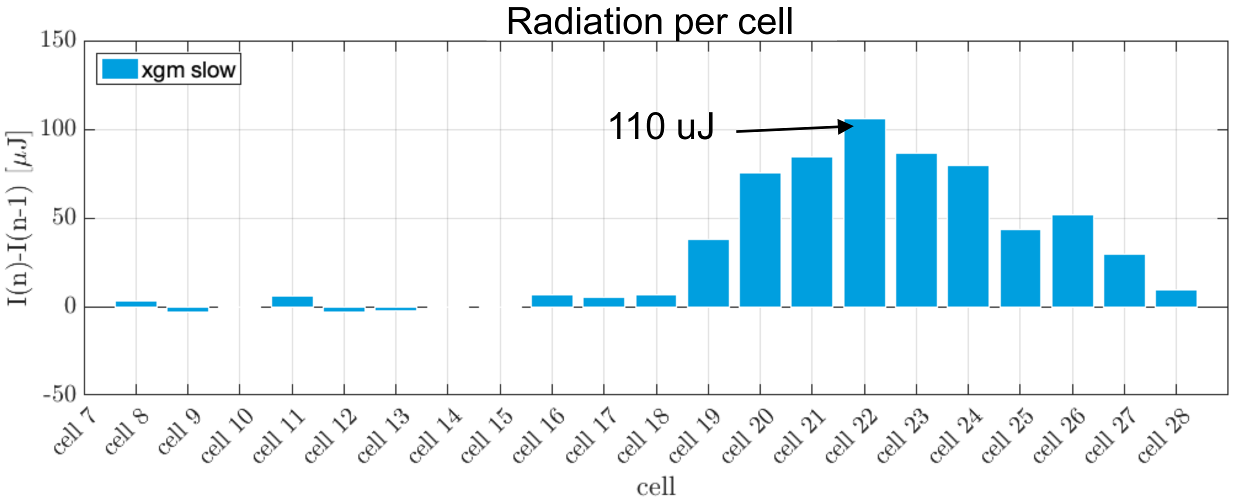
beam spot on FEL imager,
279 m behind the undulators

SA1, 24 keV, 19.10., ***400 uJ***
σx = 182 µm   σx‘ = .65 µrad
σy = 207 µm   σy‘ = 0.74 µrad



```
--- Gaussian Fit ---
amplitude-x: 519.79 +- 0.85
center-x : 1409.54 +- 0.04
sigma-x : 20.07 +- 0.04
offset-x : 15.28 +- 0.50
slope-x : -0.00 +- 0.00
amplitude-y: 487.02 +- 1.29
center-y : 559.58 +- 0.07
sigma-y : 22.76 +- 0.07
offset-y : 12.64 +- 0.79
slope-y : 0.00 +- 0.00
```

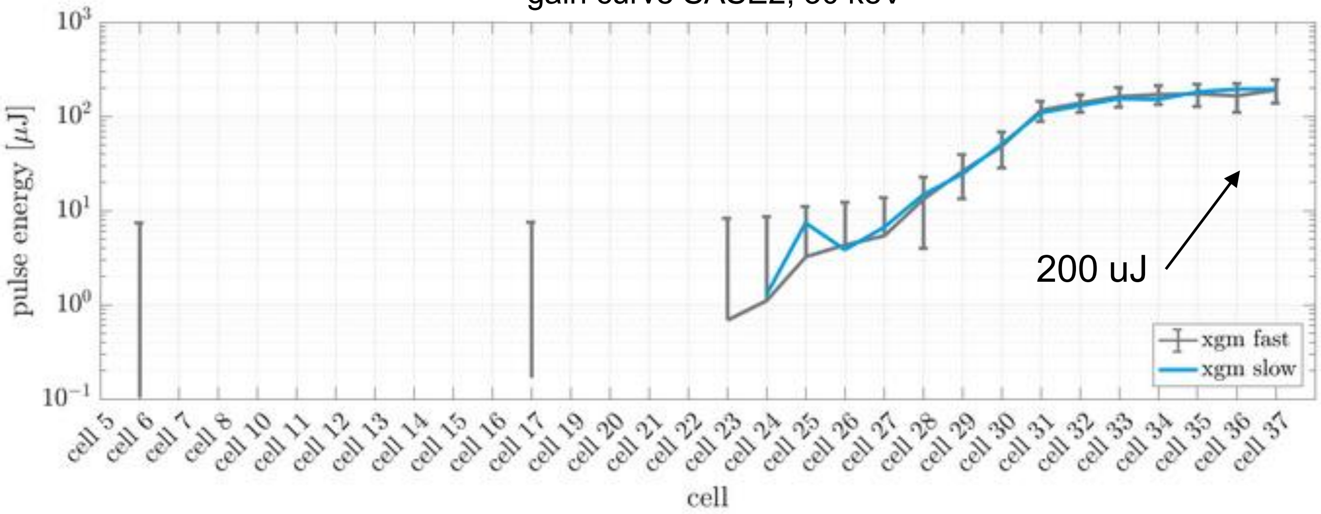




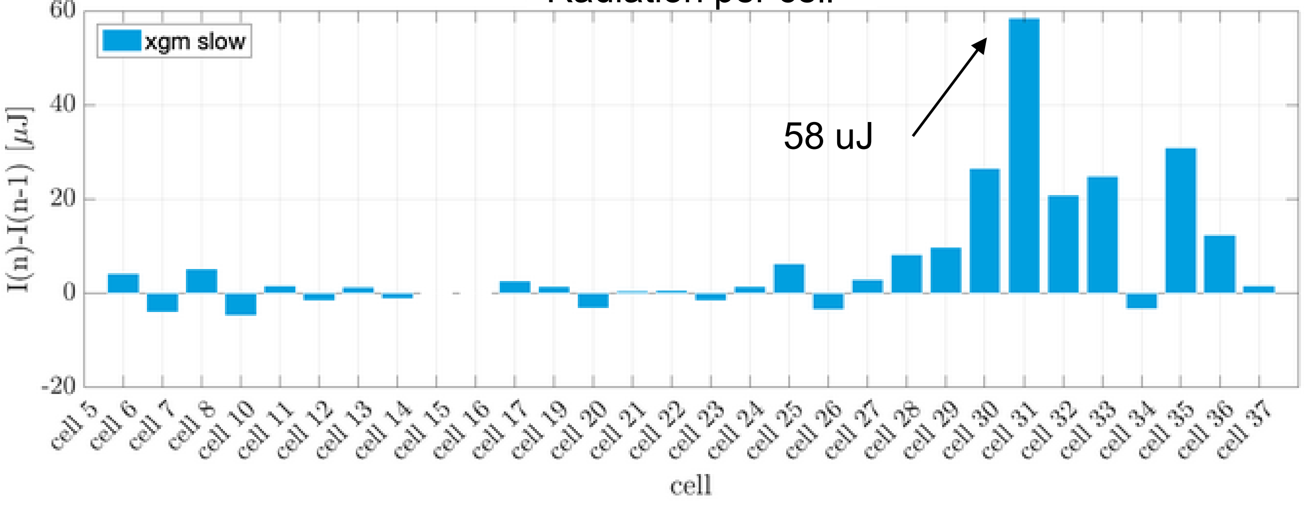
SASE2 optimization at 30 keV

- The approach was the same as for SASE1 – stepwise to 30 keV to keep some lasing alive for tuning
- Here it were the first cells which did not join the team
- The K-Mono alignment plus residual air coil optimization helped to come from ~240 µJ to ~340 µJ

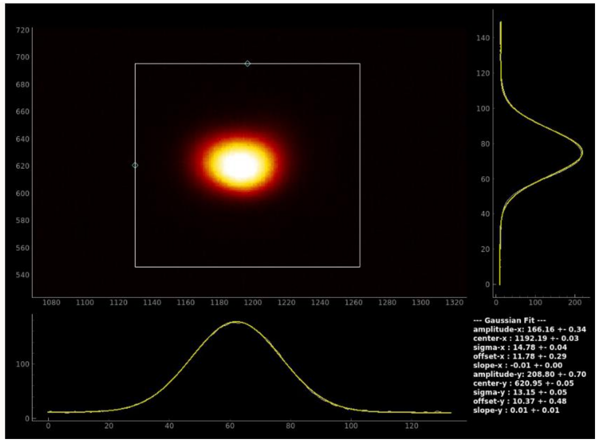
gain curve SASE2, 30 keV



Radiation per cell



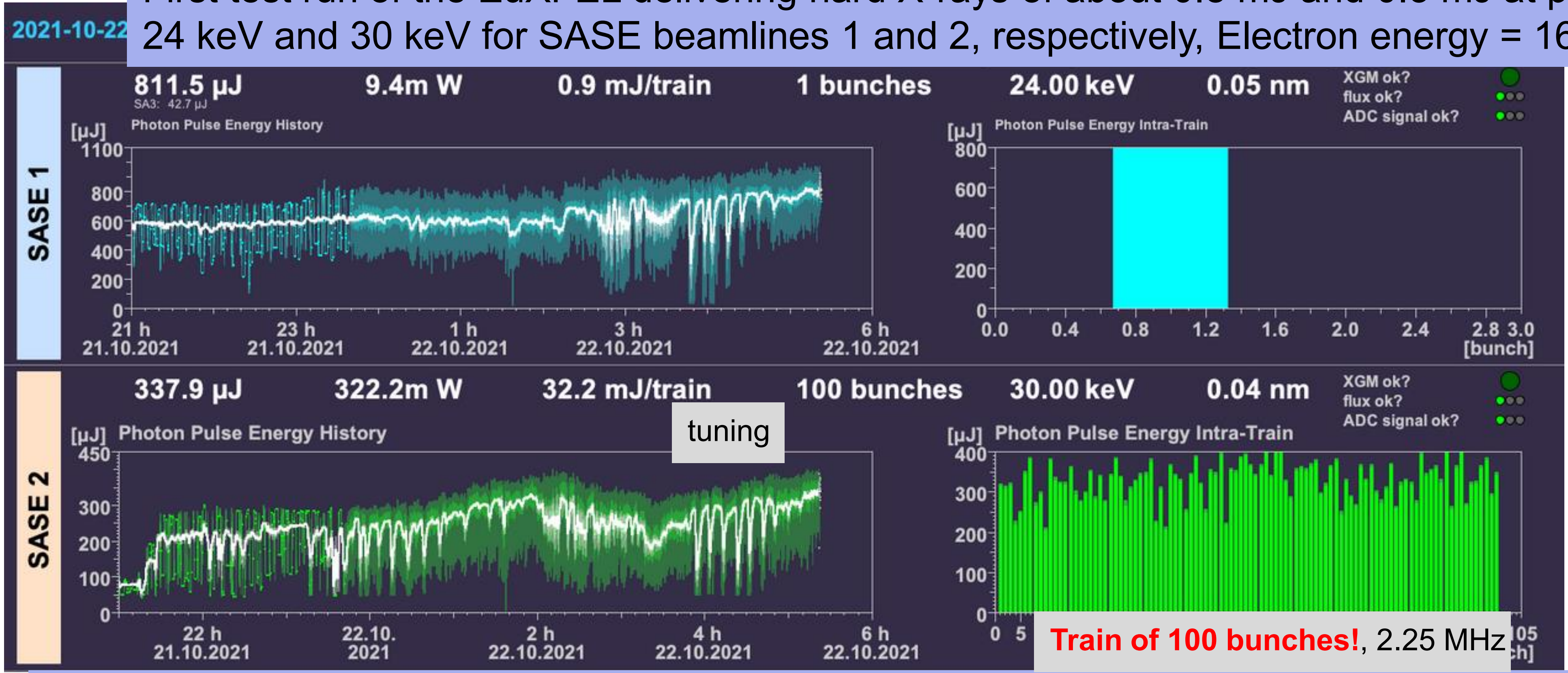
beam spot from 30 keV radiation



```
--- Gaussian Fit ---
amplitude-x: 166.16 +- 0.34
center-x : 1192.19 +- 0.03
sigma-x : 14.78 +- 0.04
offset-x : 11.78 +- 0.29
slope-x : -0.01 +- 0.00
amplitude-y: 208.80 +- 0.70
center-y : 620.95 +- 0.05
sigma-y : 13.15 +- 0.05
offset-y : 10.37 +- 0.48
slope-y : 0.01 +- 0.01
```

SA2, 30.5 keV, 21.10., 180 uJ
σx = 35 µm σx‘ = 0.60 µrad
σy = 119 µm σy‘ = 0.53 µrad

First test run of the EuXFEL delivering hard X-rays of about 0.8 mJ and 0.3 mJ at photon energies of 24 keV and 30 keV for SASE beamlines 1 and 2, respectively, Electron energy = 16.3 GeV



tuning

Train of 100 bunches!, 2.25 MHz

30 keV

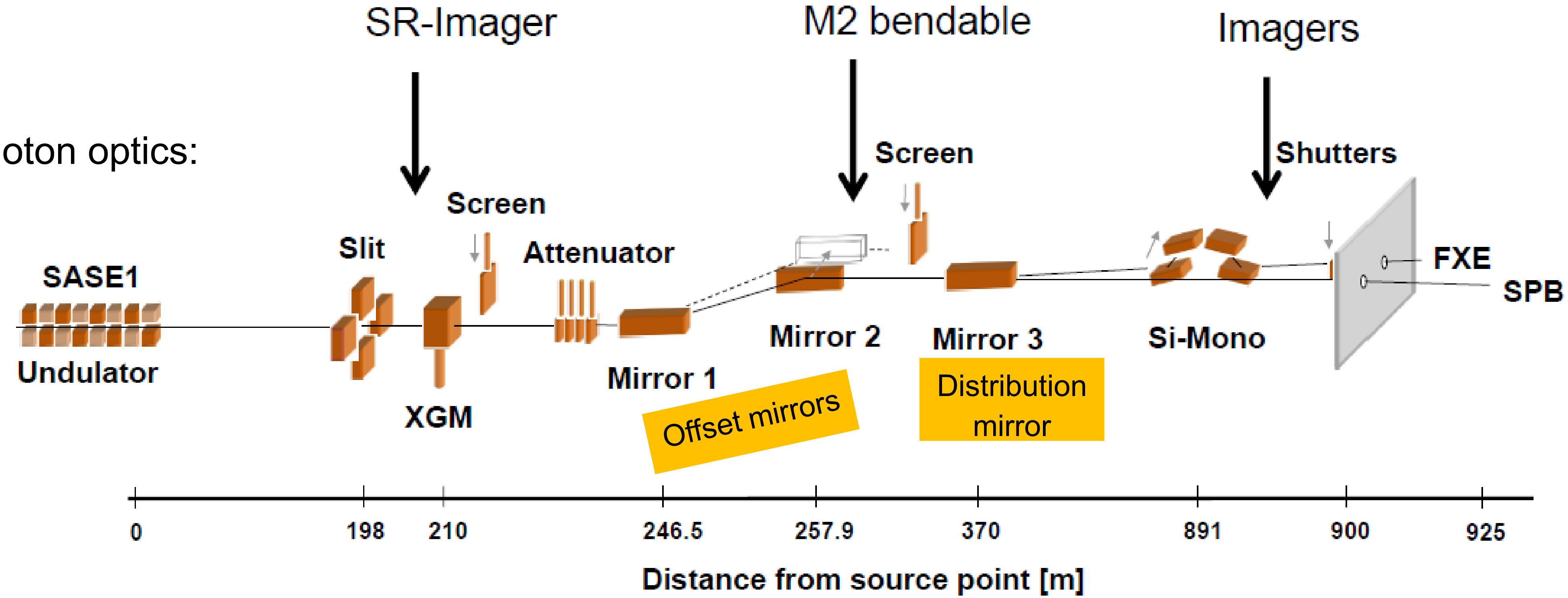
300 uJ

General experience:

- The sensitivity to all parameters is much higher
- Photon diagnostics are more noisy, but still reliable for effective tuning
- The standard tools for optimization still work (better take more bunches)
- The stability of the performance over the 3 days was great!
  - ➢ -10% and -30% w/o further tuning

Next step: Can we get the photons to the experiments?

Photon optics:



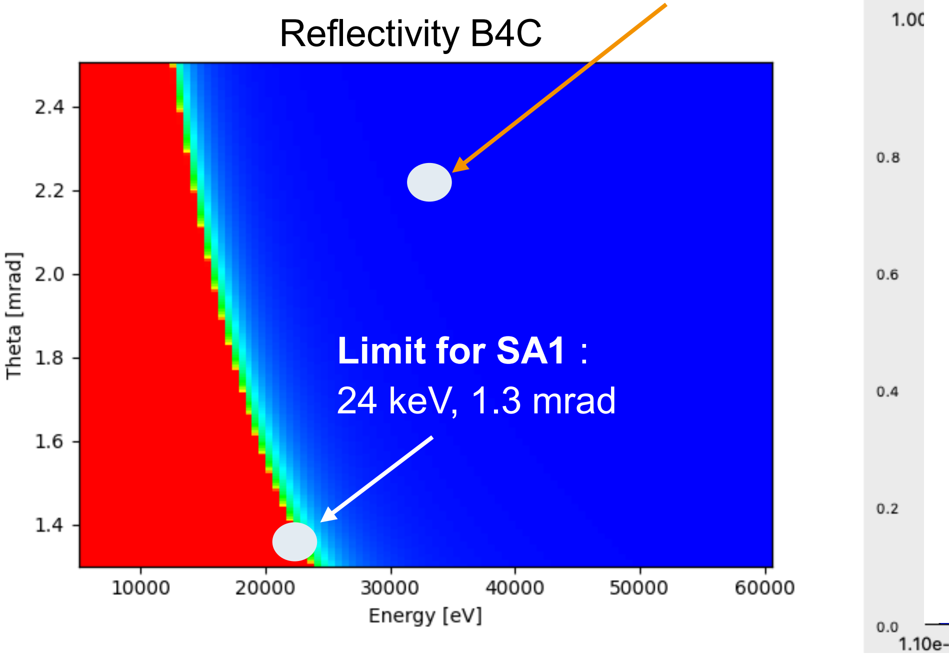
Super polished mirrors

- Photons are guided over 2-3 mirrors
- Incident angles > 1.3 mrad

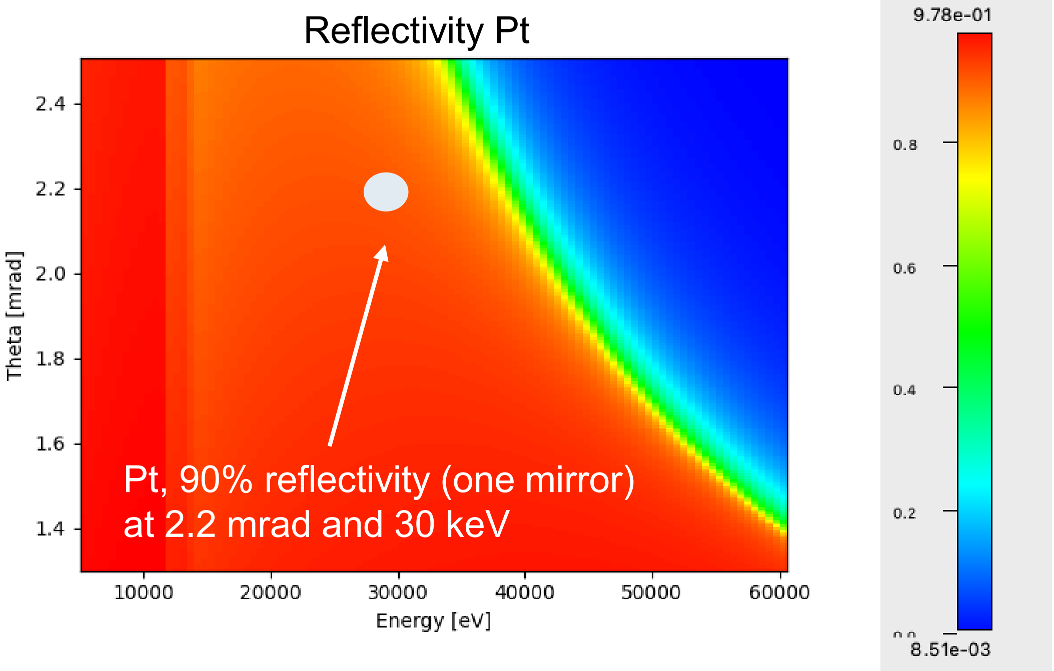
Reflectivity ?

Reflectivity of mirrors for different coatings, B4C vs. Pt

B4C, 0.4% reflectivity (one mirror) at 2.2 mrad and 30 keV


Reflectivity B4C

Limit for SA1 :
24 keV, 1.3 mrad


Reflectivity Pt

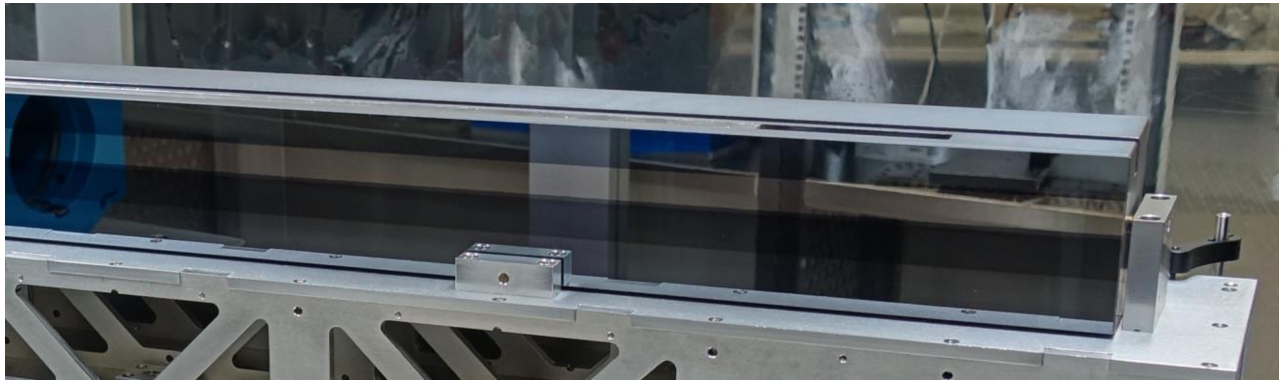
Pt, 90% reflectivity (one mirror)
at 2.2 mrad and 30 keV

For > 24 keV the platinum coating allows to extend the energy range.

The minimal incident angle is 1.3 mrad, defined by the footprint of the radiation

Super polished mirror with
B4C and Pt stripes

Only available at SASE 2

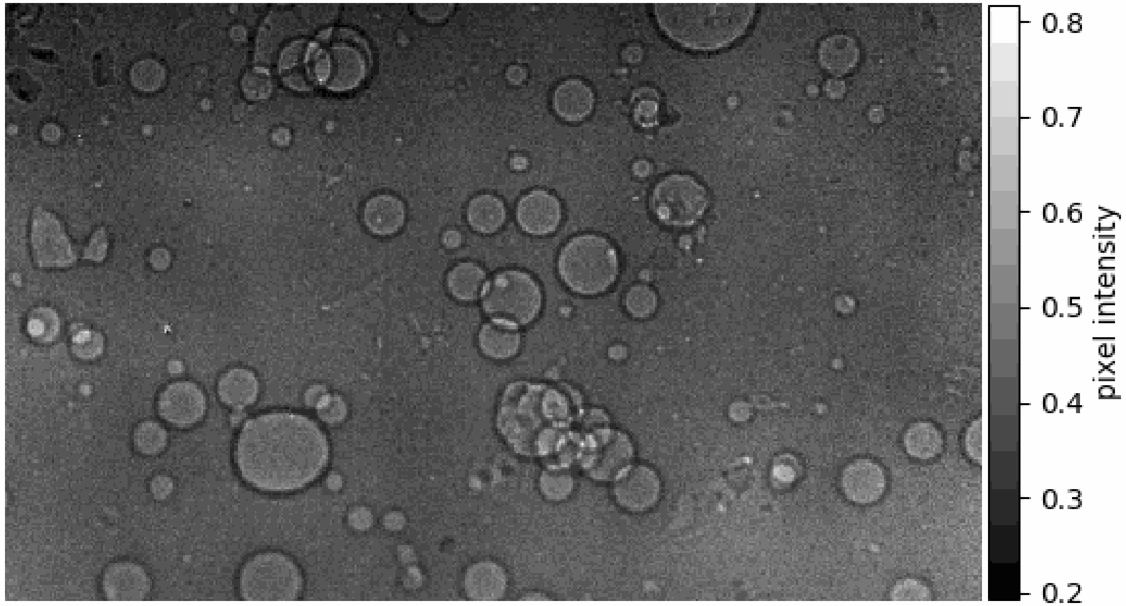


X-Ray microscopy at 24 keV, SASE 1

- At SASE 1 the 24 keV photons could be guided to the SPB hutch and first experiments have been done over the weekend.
- At SASE 2 we started later and at the end the 30 keV beam vanished somewhere in the beamline

So we had to repeat this of course…

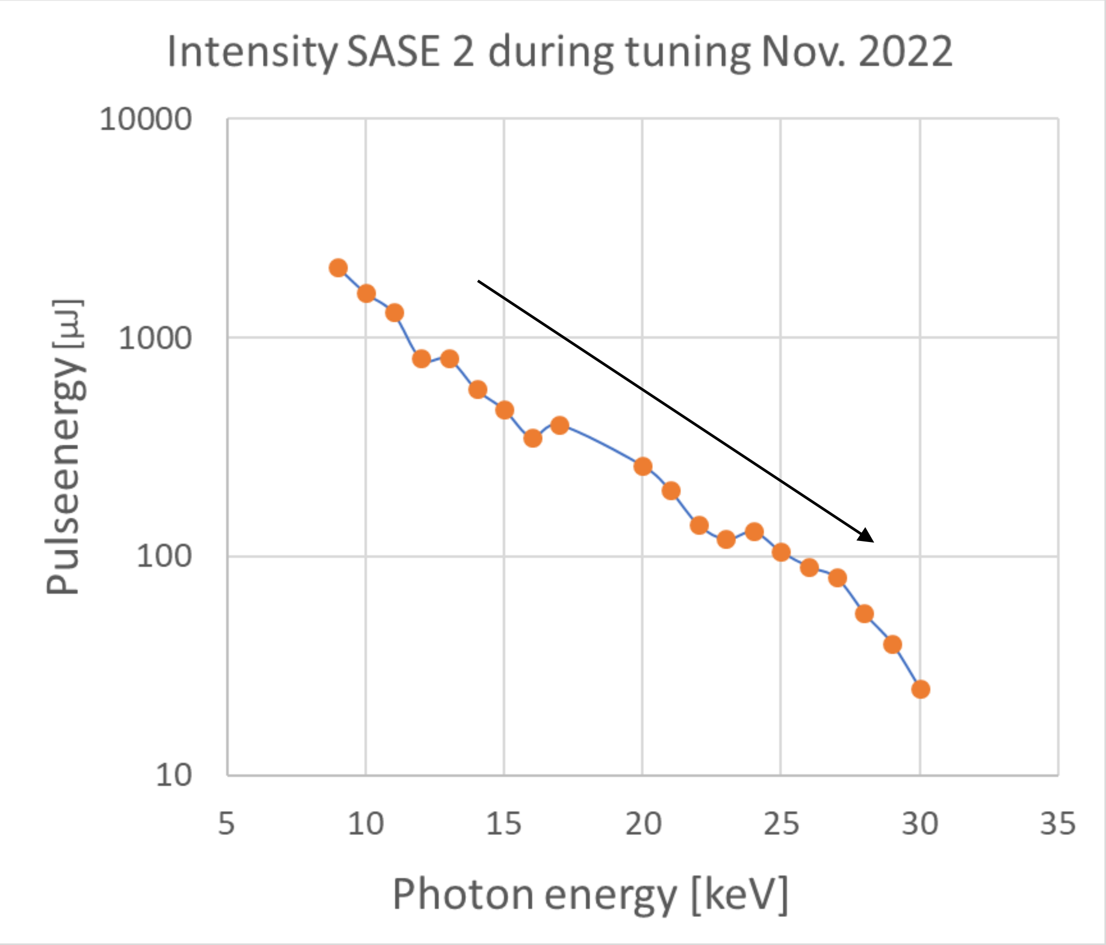
Early foaming in Al in slow motion
Recorded at SPB EuXFEL, P.Vagovic



Courtesy of Meik Noak and Francisco Garcia-Moreno, TU Berlin

Results from the second attempt with 30 keV, Nov 23th – 26th 2022:

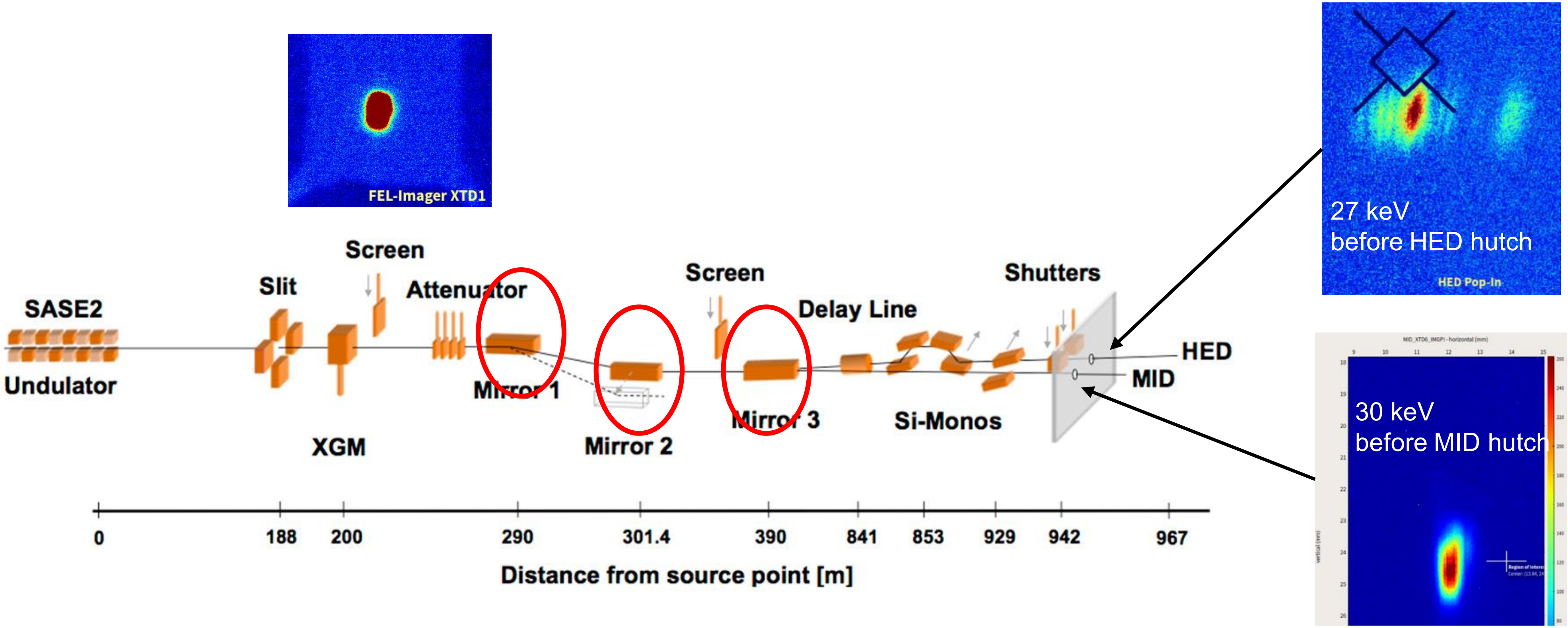
- Priority this time on the **photon transport SASE 2**
- Electron energy 16.5 GeV
- Spending less time on tuning – low intensities
- ***Only about 20-40 µJ at 30 keV***



Successful transmission to SASE 2, MID and HED

This time we did a stepwise approach starting at to 20 keV where the transmission could be found rather quick and then increasing the energy stepwise while the EuXFEL optics group tuned the alignment. [M. Vannoni et.al.]
After this, transport up to the experiment was done with a transmission of

- About 60% at 27 keV
- About 40% at 30 keV (large uncertainty due to low signal / large background, max. possible $90\%^3 = 73\ \%$)



How can we extend the energy range further?

1. With the present undulators
    - Reduce emittance and energy spread
    - Optimize beta function
    - Reduce distortions within the undulator beamline
        - Straight trajectory
        - Undulator positions
        - Kicks from undulators and phase shifters
        - Compensation of ambient fields
2. With additional short period undulators (after burner)
    - Superconducting undulators allow shorter periods and strong fields with a large flexibility
3. With harmonic lasing
4. With new undulators (not covered from this talk)
    - The optimum for the high energy goal would be a complete beamline with short period undulators
    - This implies a limitation for the lowest possible energy

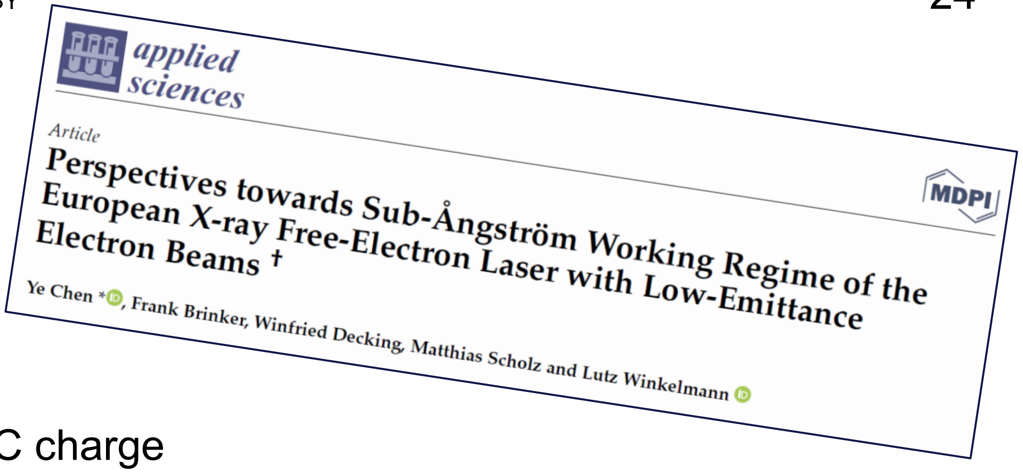
Laser shaping, compression
optimization

e-Beam based alignment
photon based alignment
+ empirical tuning

Future developments:

- Improved beam properties
- After burner, SC undulators
- Harmonic lasing

What can we expect with improved emittances?



applied sciences

Article

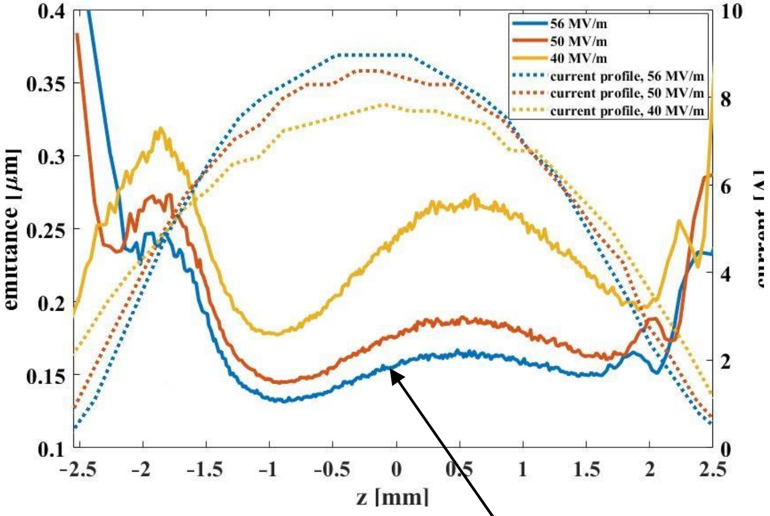
Perspectives towards Sub-Ångström Working Regime of the European X-ray Free-Electron Laser with Low-Emittance Electron Beams †

Ye Chen *, Frank Brinker, Winfried Decking, Matthias Scholz and Lutz Winkelmann

With optimized ***transverse cathode laser shapes*** significantly reduced emittances should be possible.

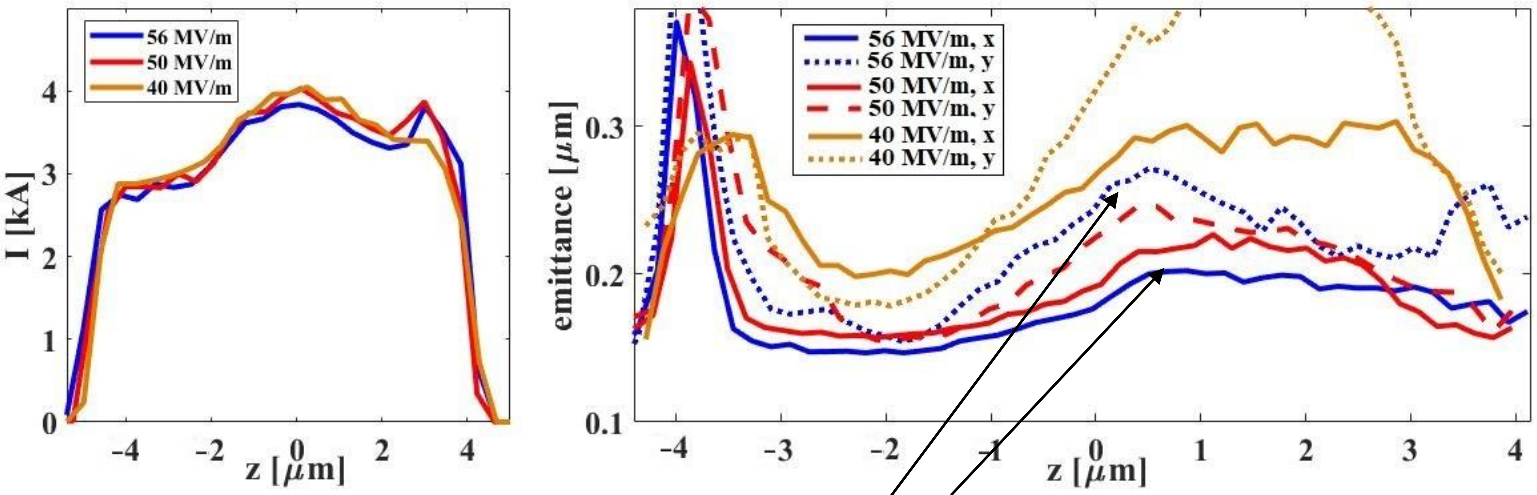
Electron bunch profiles for a gun gradient of 40, 50, 56 MV/m with 100 pC charge

Injector



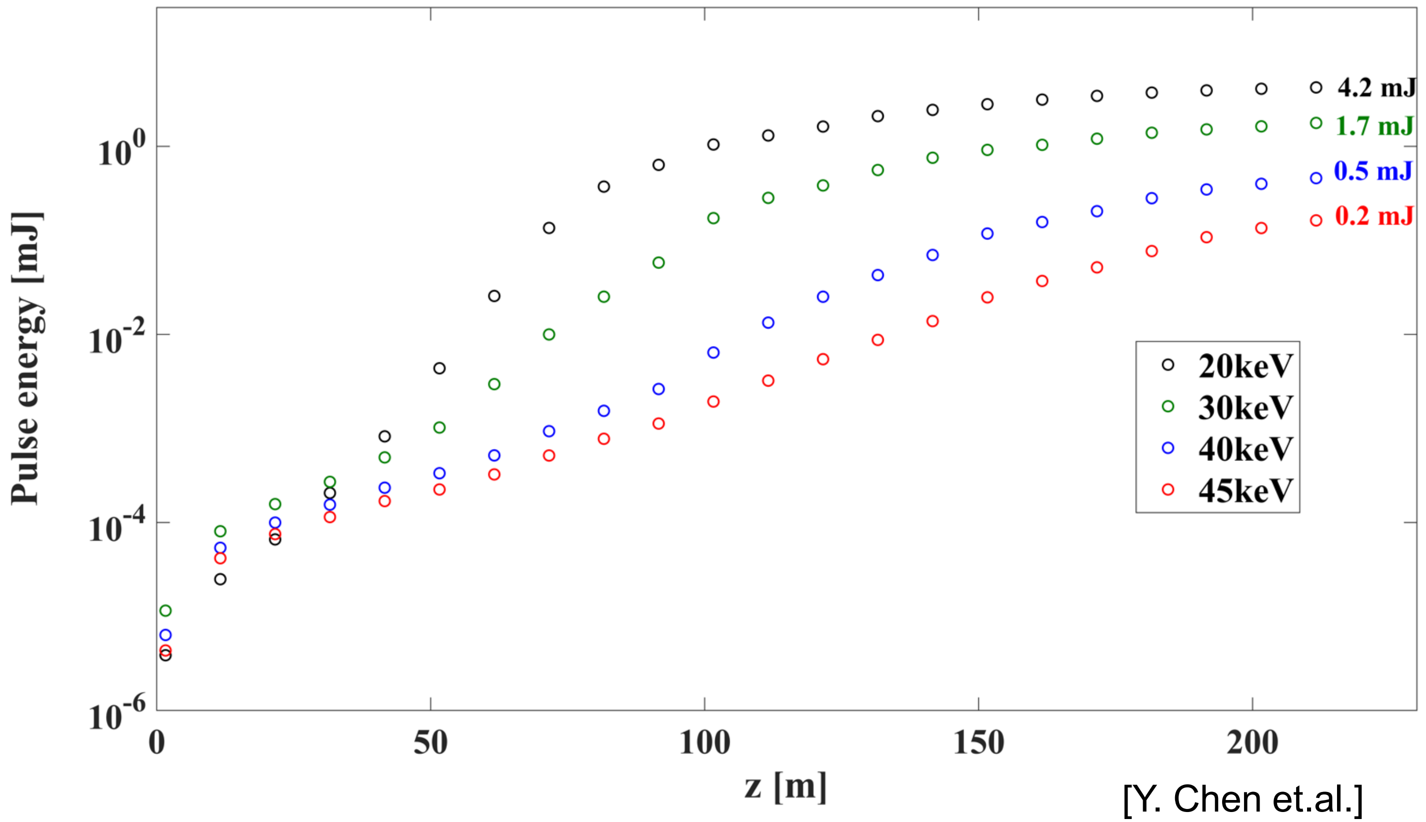
ε(slice) = ~0.16 μm

At the undulators



ε_x(slice) = ~0.22 μm, ε_y(slice) = ~0.25 μm

Projected intensities assuming a low emittance beam with low energy spread and *perfectly aligned* undulator sections



[Y. Chen et.al.]

Photon energy	Wave length	Power / pulse
20 keV	0.62 Å	4.2 mJ
30 keV	0.41 Å	1.7 mJ
40 keV	0.31 Å	0.5 mJ
45 keV	0.28 Å	0.2 mJ

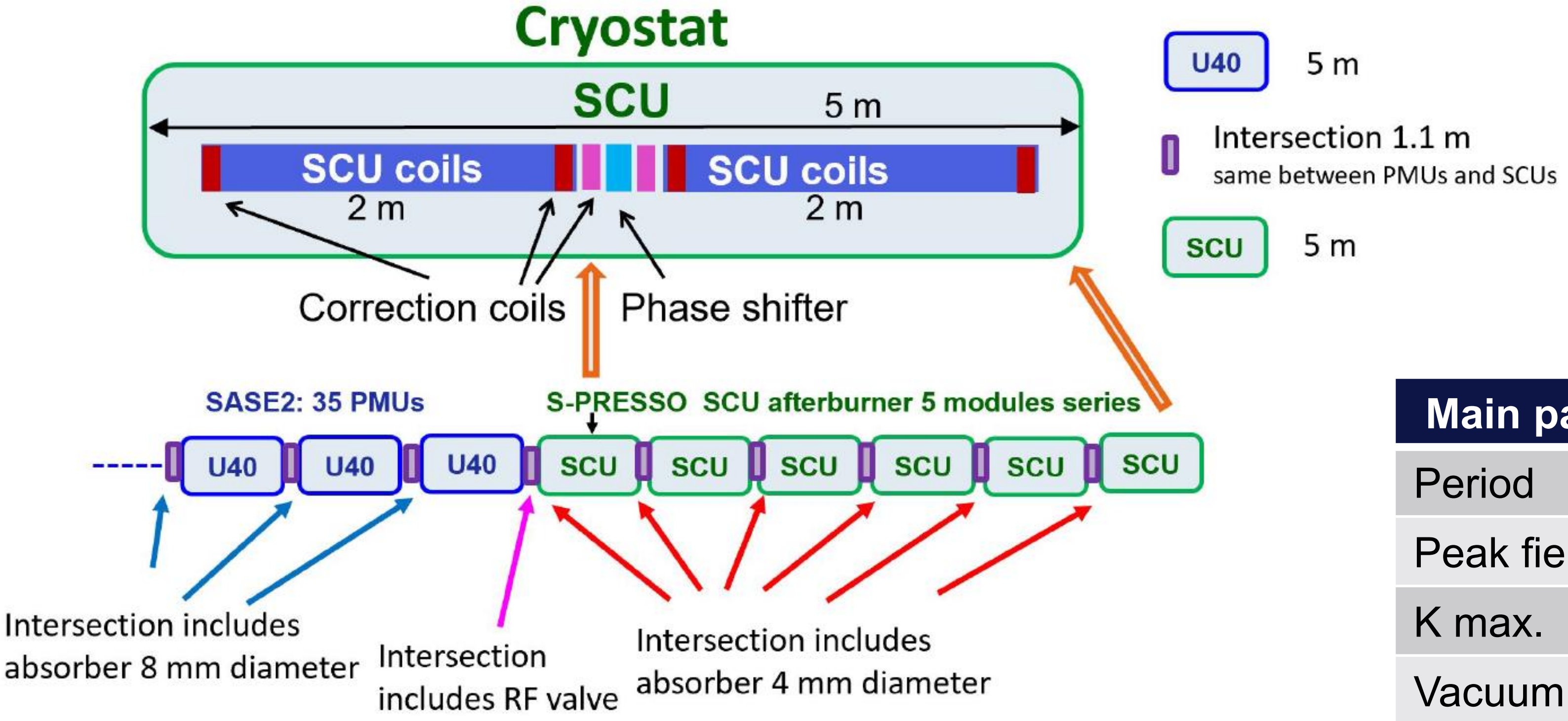
Electron energy = 17.5 GeV
Bunch charge = 100 pC
Emittance = 0.25 mm mrad
Gun gradient = 56 MV/m
Energy spread = 2.0 MeV
35 cells with 5m undulators

At 40 and 45 keV the undulator length is not sufficient to reach full saturation.

Future developments:

- Improved beam properties
- Afterburner, SC undulators
- Harmonic lasing

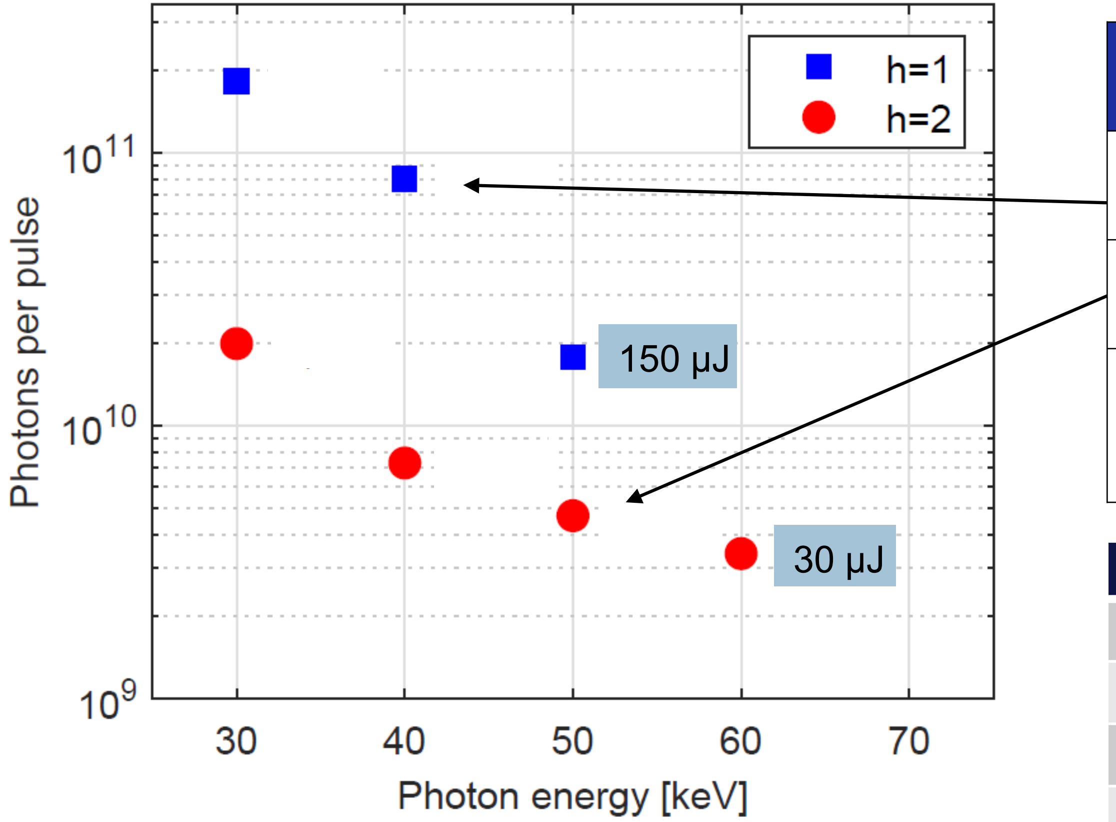
Next Step: *The super conducting afterburner*



S-PRESSO, the prototype of the super conducting undulators has been ordered and is expected for end of 2024. [S.Casalbuoni, et. al. 2022]

Main parameter	PMU	SCU
Period	40 mm	18 mm
Peak field	1.12 T	1.82 T
K max.	3.93	3.06
Vacuum chamber	8 x 40 mm	5 x 10 mm
Magnetic length	5 m	4 m

Possible scenarios for the afterburner using the fundamental and 2nd harmonic :



Setup for lasing at wavelength λ	Effect	gain
All undulators set to λ	Additional undulators with larger K	Higher intensity
PMUs set to 2 λ SCUs set to λ	Nonlinear harmonic generation – 2nd harmonic	Extended energy range
PMUs set to 3 λ SCUs set to λ	Amplifying the 3rd harmonic of the radiation	Extended energy range

Electron parameter for the simulation	
Energy	16.5 GeV
Norm. emittance	0.4 mm mrad
Initial Energy spread	3 MeV
Peak current	5 kA
Bunch charge	150 pC
bunch length	30 fs

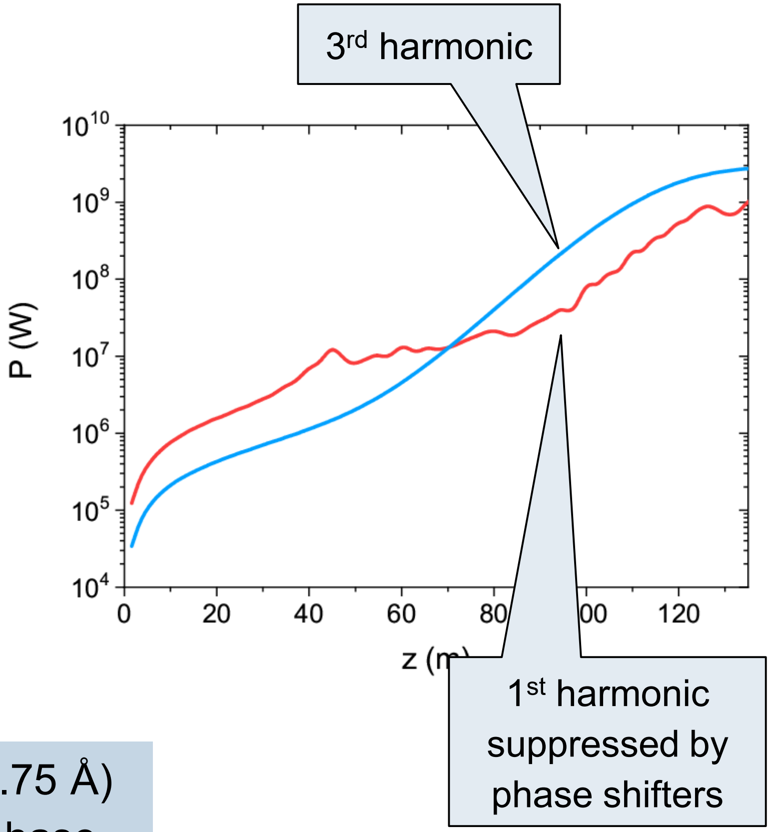
Simulations with 24 m SCUs after the SASE2 undulators.
N1 = No of active PMUs [C. Lechner et.al. 2022]

Future developments:

- Improved beam properties
- After burner, SC undulators
- Harmonic lasing

Lasing on the 3rd harmonic

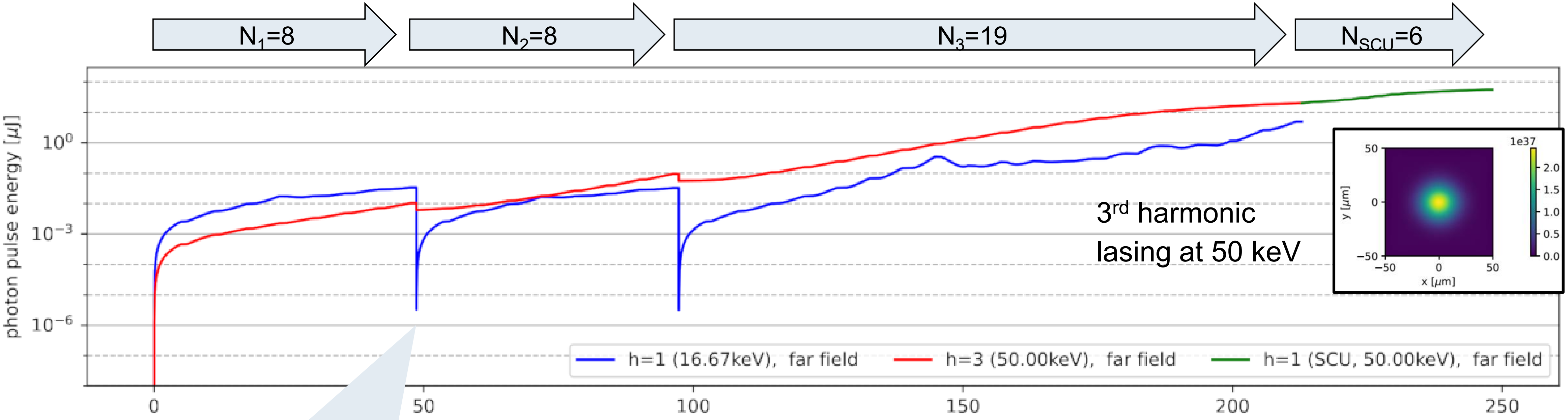
- Harmonic lasing on the odd harmonics of the fundamental wavelength develops independently of the fundamental
- The fundamental lasing has to be disrupted to keep the energy spread low and let the harmonic saturate
- In order to preserve the beam quality for the SCUs the development of the first harmonic radiation has to be suppressed by two methods:
  - Insertion of filters for the fundamental wavelength
  - Setting the phase shifters between the undulators to $2\pi/3$, $4\pi/3$ to get destructive interference for the fundamental [E. Schneidmiller et.al., 2012]



This scheme has been demonstrated at the soft X-Ray beamline SASE 3 at 4.5 keV (2.75 Å) using the 3rd harmonic of 1.5 keV and 5th harmonic of 0.9 keV in 2019/2020 using the phase shifters to suppress the fundamental and last 6 cells set to the fundamental.

Example for 50 keV 3rd harmonic lasing using the super conducting afterburner

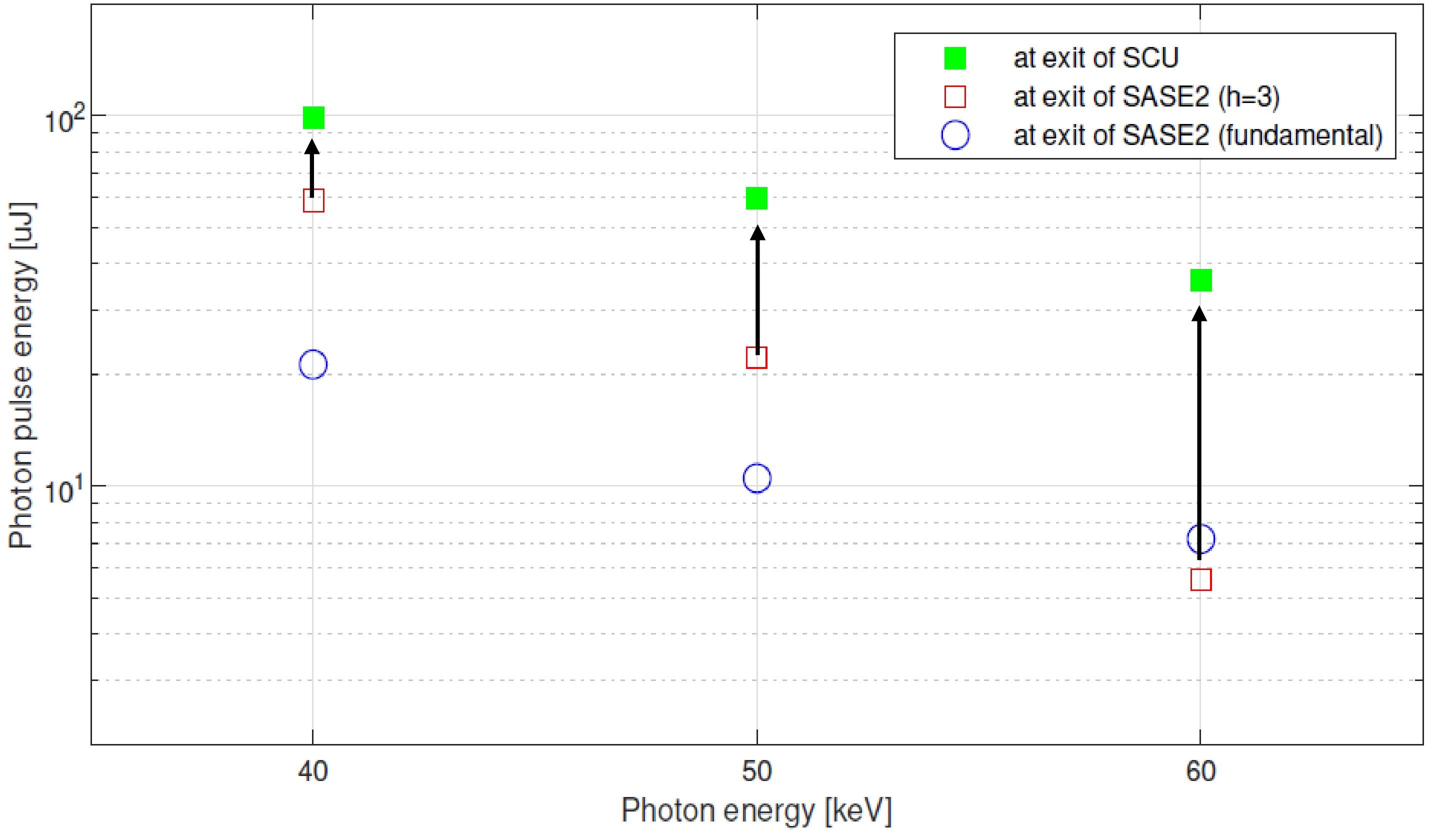
Recent simulations show the evolution of the Photon pulse energy in SASE2 at the **fundamental wavelength (blue)** and at the **third harmonic (red)**, respectively, and in the **SCUs (green)** tuned to the third harmonic of SASE2. [C.Lechner et.al., 2023]



3^{rd} harmonic
lasing at 50 keV

Disruption of the fundamental by a Si filter using the self seeding chicanes in SASE 2

Intensity boost from the SCU afterburner



Photon pulse energies after SASE 2 and after the SCUs

Summary

- Due to the possibility to accelerate electrons up to 17.5 GeV the European XFEL is best suited to produce laser light at extremely high photon energies
- Already now experiments with up to 24 keV are offered and realized
- Discussions with the user community, like the recent workshop, show a growing demand to extend the energy range even further
- A step wise approach is outlined to proceed in that direction:
  - With the present hardware the energy range could be extended to 30 keV showing the capability of the accelerator the photon optics and the photon diagnostics to handle this
  - The planned super conducting afterburner would bring the intensities at these energies to a new level and/or would extend the wavelength range
  - New schemes like harmonic lasing, especially in connection with the afterburner promises a new approach

Thank you for your attention

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