Stable and Brilliant Self-Seeded XFEL at SACLA

Ichiro Inoue

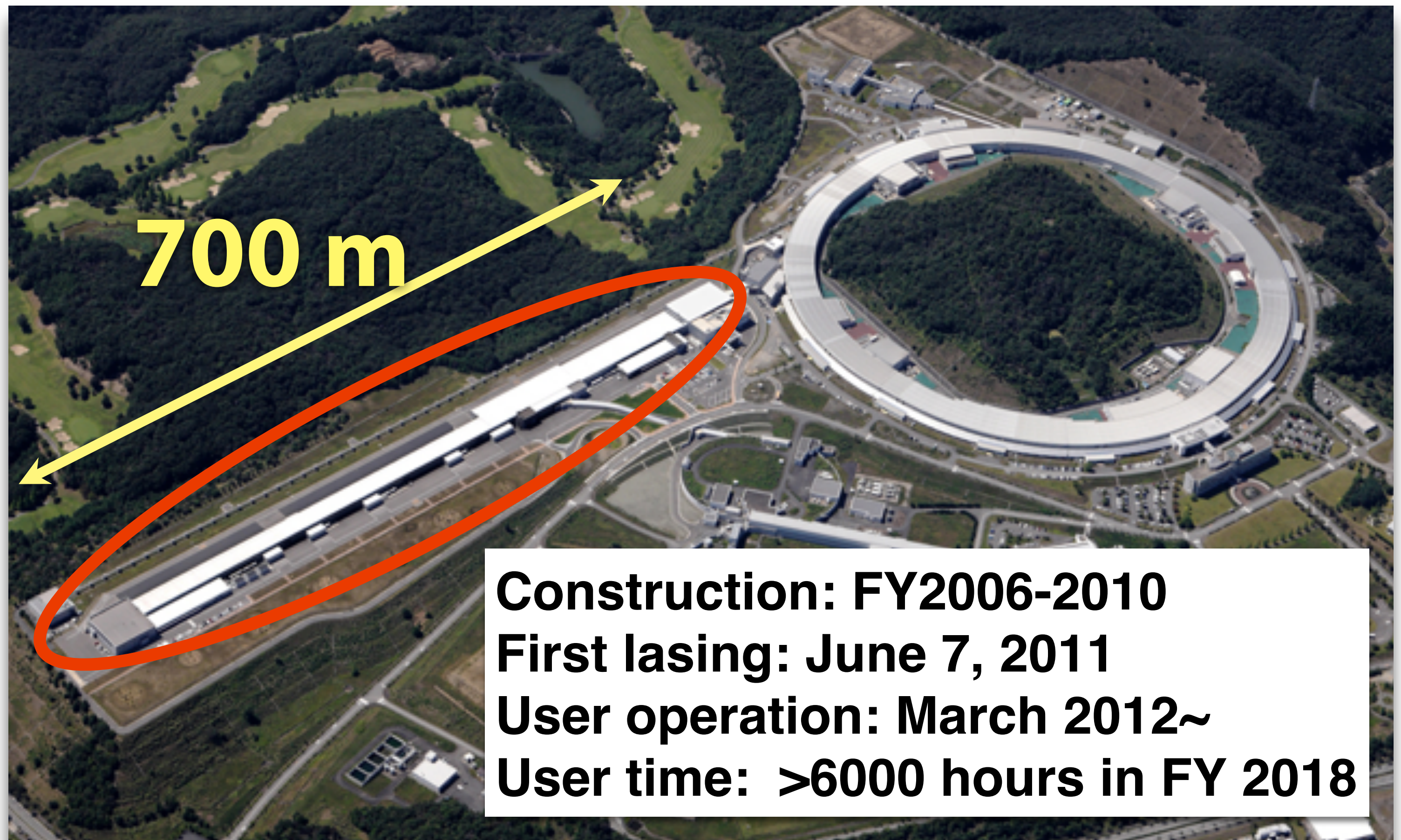
RIKEN SPring-8 Center/SACLA

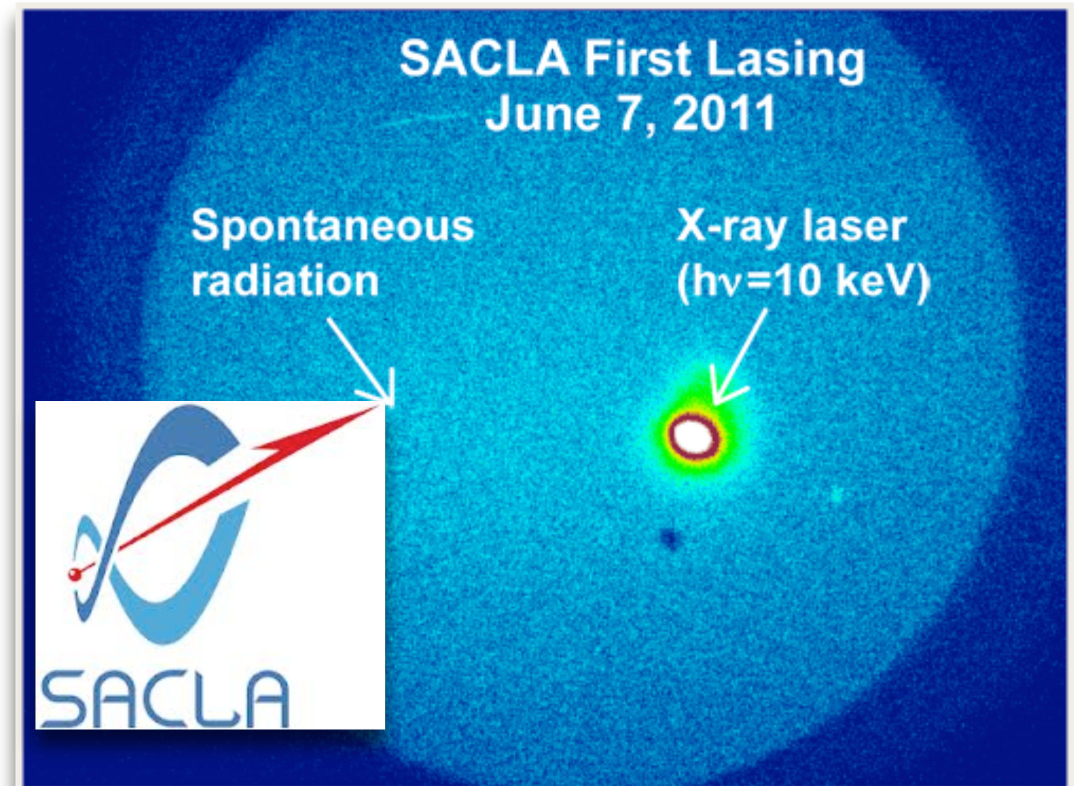
On behalf of SACLA accelerator and beamline teams

Contents

- Brief introduction of SACLA
- Background & concept of reflection self-seeding
- Early commissioning results
- Recent progress & future perspectives

SPring-8 Angstrom Compact free-electron LAser "SACLA"





LETTERS

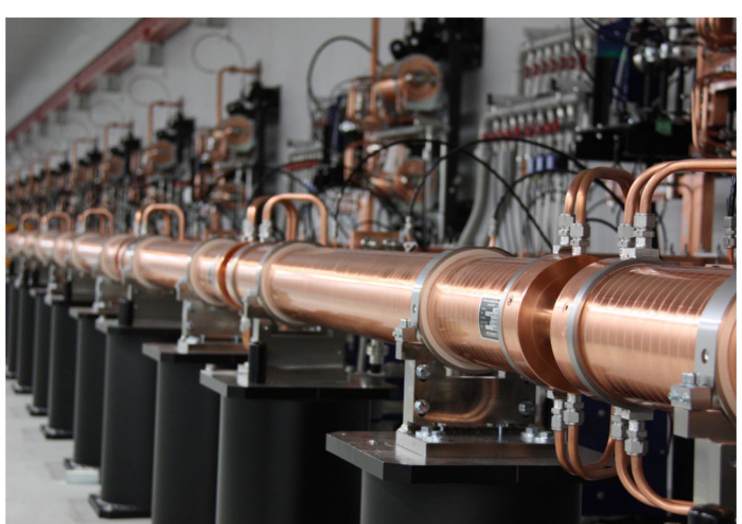
PUBLISHED ONLINE: 24 JUNE 2012 | DOI: 10.1038/NPHOTON.2012.141

nature photonics

A compact X-ray free-electron laser emitting in the sub-ångström region

Hitoshi Tanaka and Makina Yabashi *et al.**

High gradient C-band accelerator (acceleration gradient: 35 MV/m)

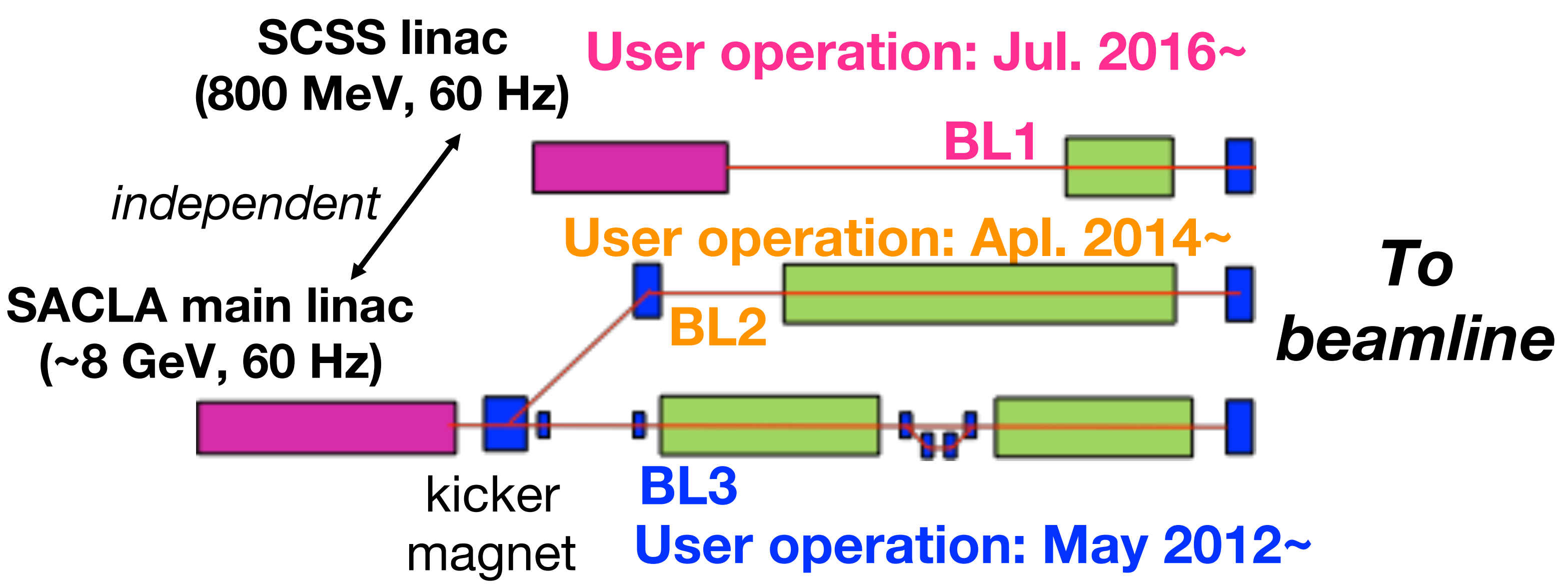


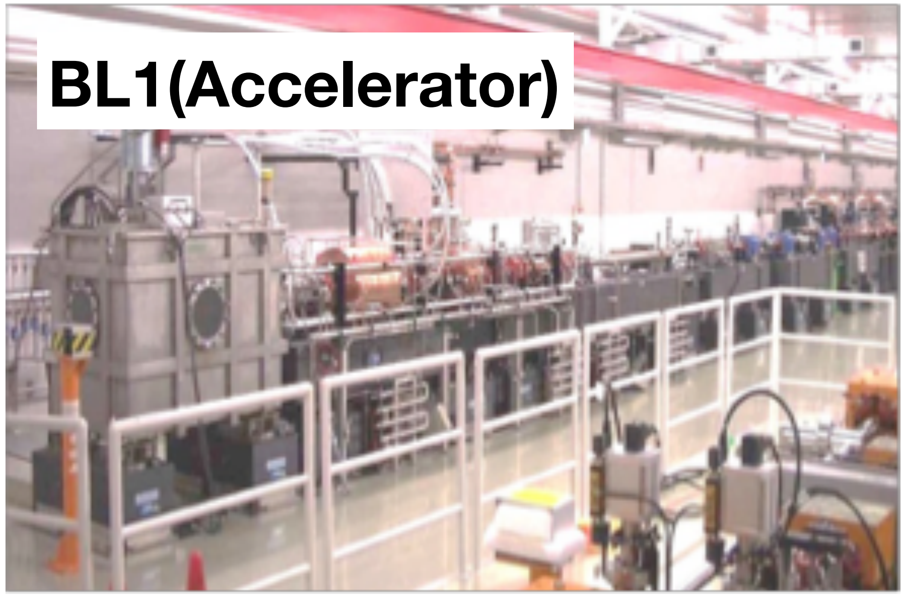
In-vacuum short period undulator (λ_u=18 mm)

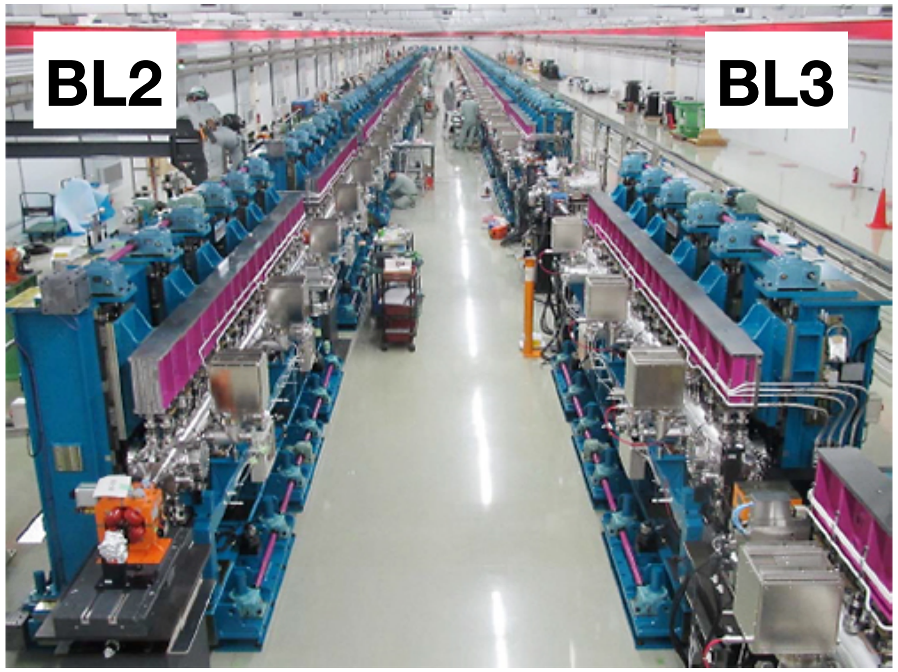
XFEL amplification can be achieved at a relatively short distance (~700 m)

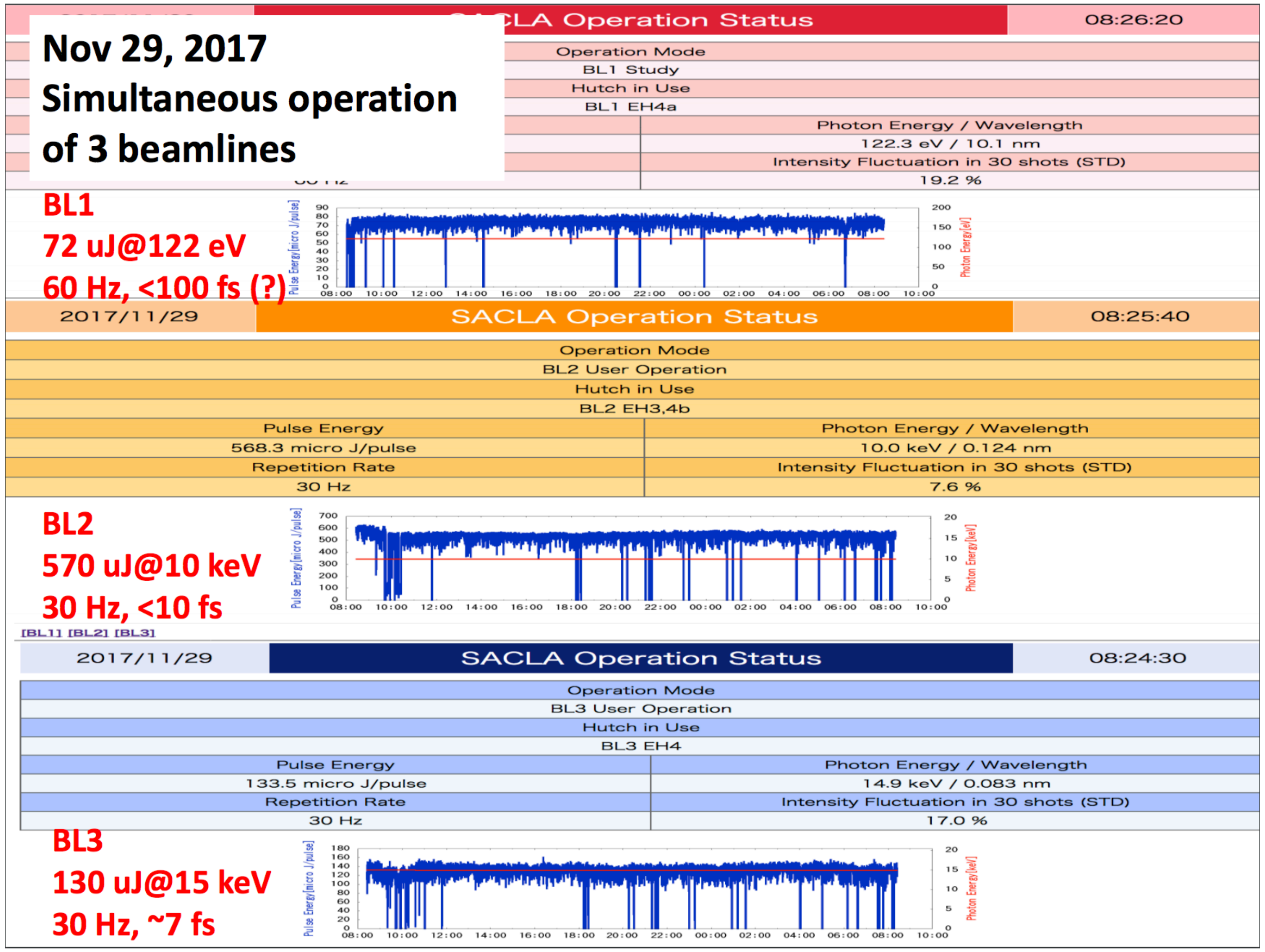
Accelerator and undulators of SACLA

Accelerator & undulators



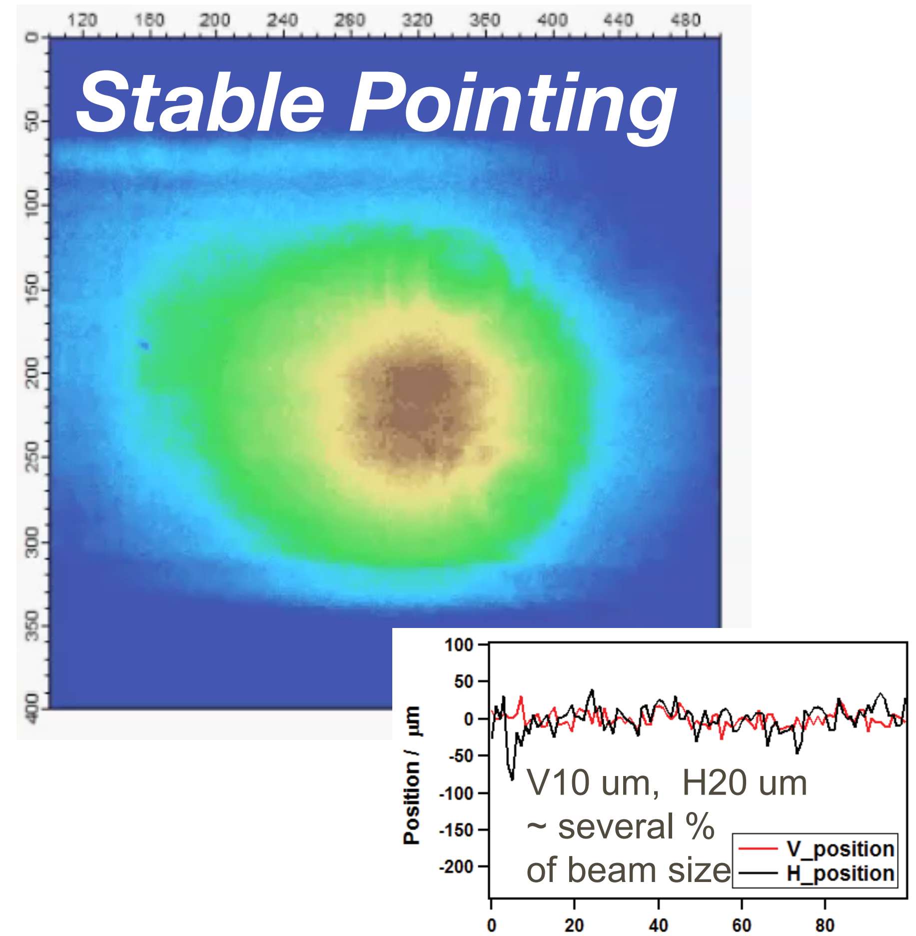




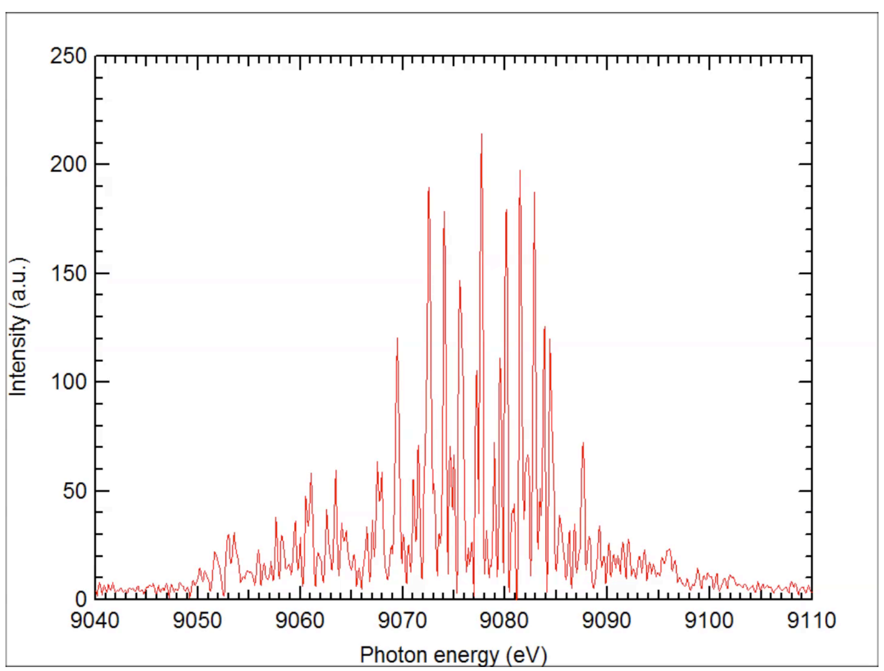


XFEL properties of SACLA (BL2&BL3)

Photon energy & Photon number (Pulse energy)	4—15 keV >10^{11} photons/pulse (max. 600 μJ)
Pulse duration	<10 fs
Peak power	>60 GW @ 10 keV
Rep. rate	Max. 60Hz
Band width: Pink	~5×10^{-3} plane mirrors
Monochromatic	~1×10^{-4} Si(111)
Coherence length	Almost the same as beam size

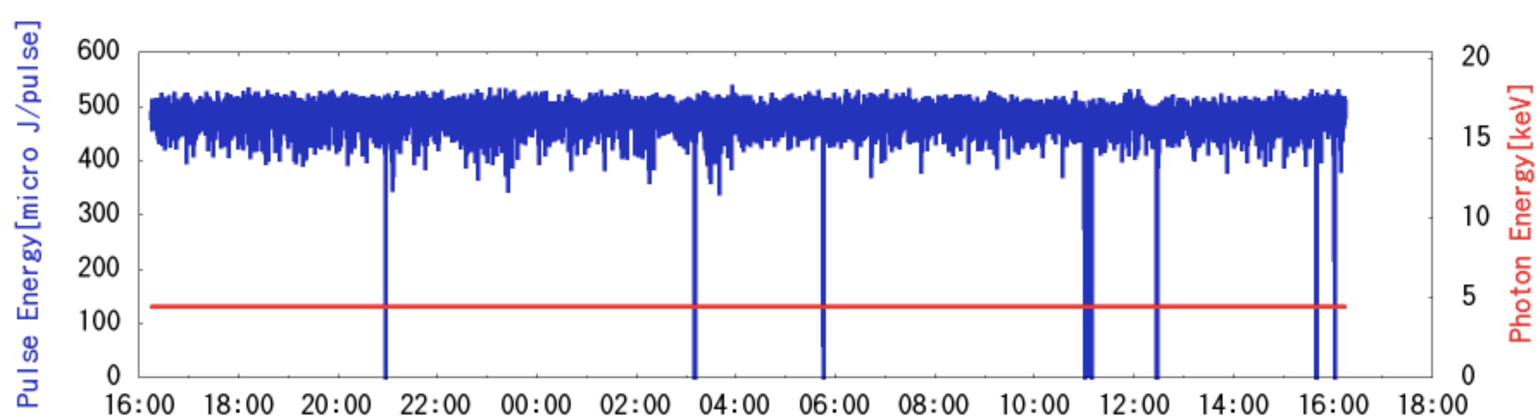


Stable Spectrum



Stable Operation

Pulse Energy	Photon Energy / Wavelength
509.2 micro J/pulse	4.4 keV / 0.279 nm
Repetition Rate	Intensity Fluctuation in 30 shots (STD)
60 Hz	11.1 %



Fluctuation of center of photon enargy: 10 eV (STD)

Photon energy spread of each pulse: ~15 eV (STD)

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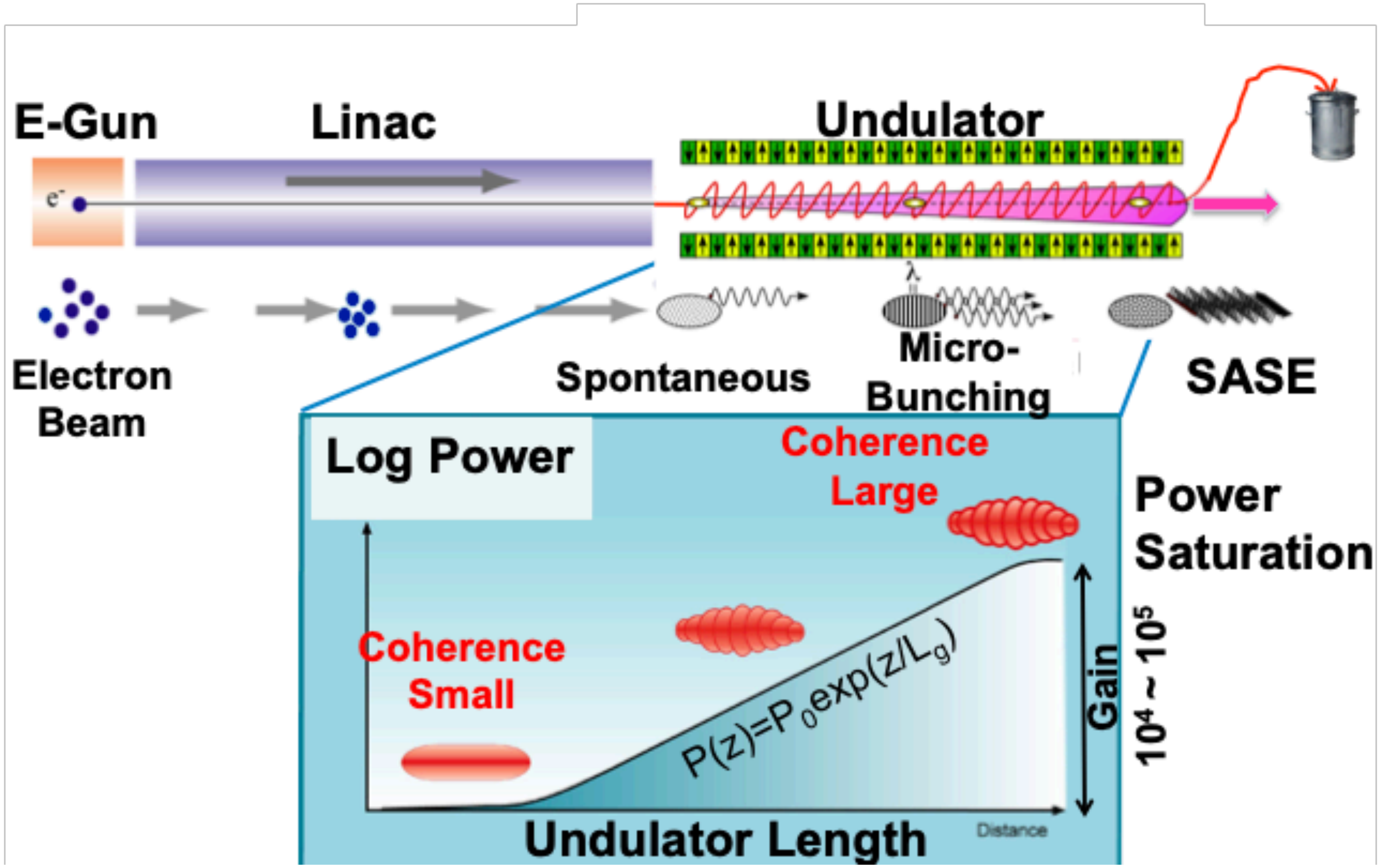
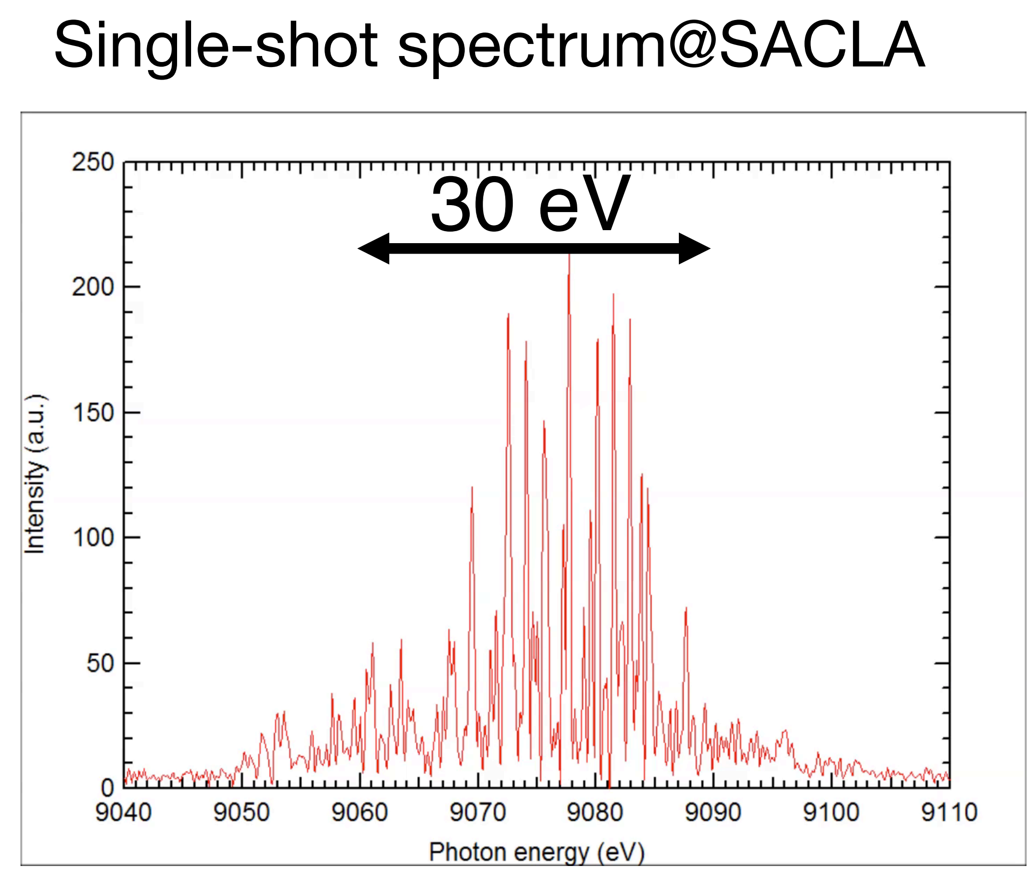
Principle of single-path FELs





Y. Inubushi, *Appl. Sci.* (2017).

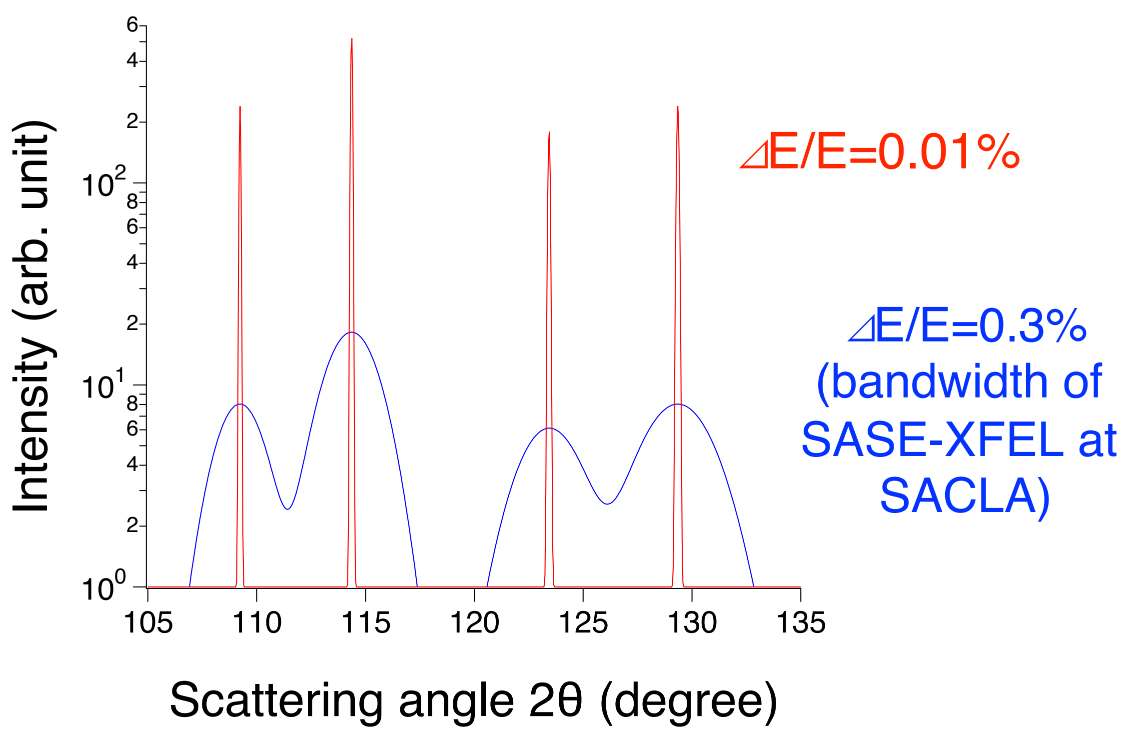
Amplification processes start from undulator radiation with broad bandwidth→ XFEL beam has relatively large bandwidth (⊿E/E~0.3%)

Why we need narrow-band XFELs ?

Reason I:
some experiments cannot be performed with pink beam (⊿E/E~0.3%)

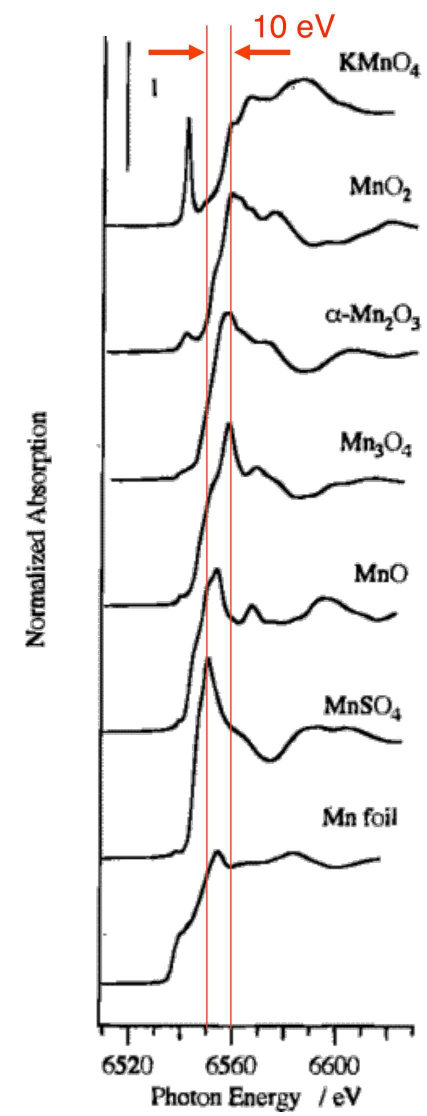
Example 1: Wide angle diffraction

e.g. Diffraction intensity profile of silicon (Simulation)



Diffraction lines are spatially overlapped when pink beam is used,
-> makes detailed structure analysis impossible

Example 2: Spectroscopy



Mn K-edge absorption spectrum for various manganese compounds

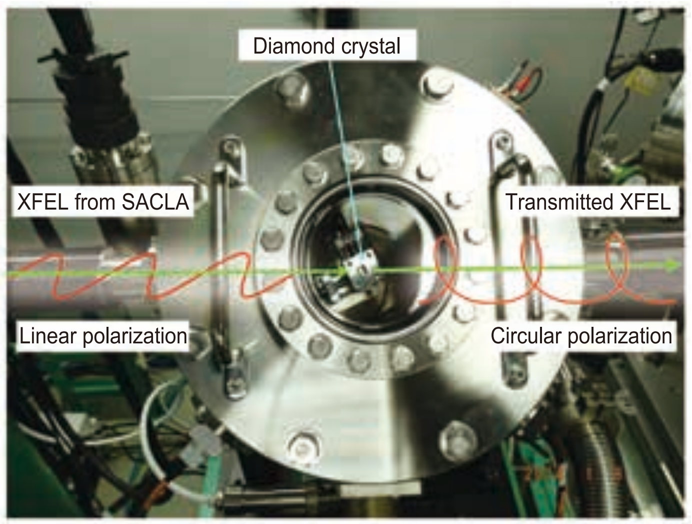
The bandwidth of incident X-ray beam should be a few eV or less

Yamamoto *et al.*,
J. Phys. Chem. B 103, 2385 (1999)

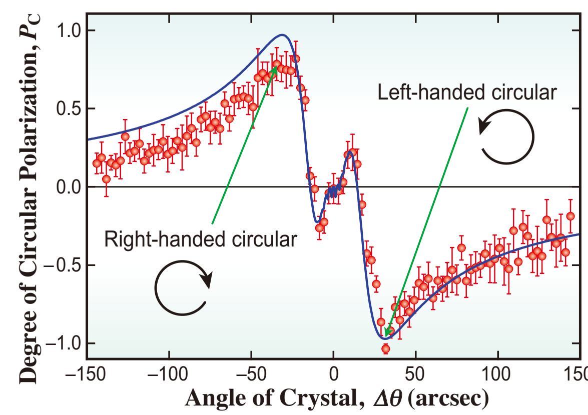
For performing these experiments, SASE-XFEL beam should be monochromatized at the cost of considerable loss of photon flux

Why we need narrow-band XFELs ?

Reason II:
Crystal optics are used everywhere at XFEL facilities, and most of them utilize Bragg reflection

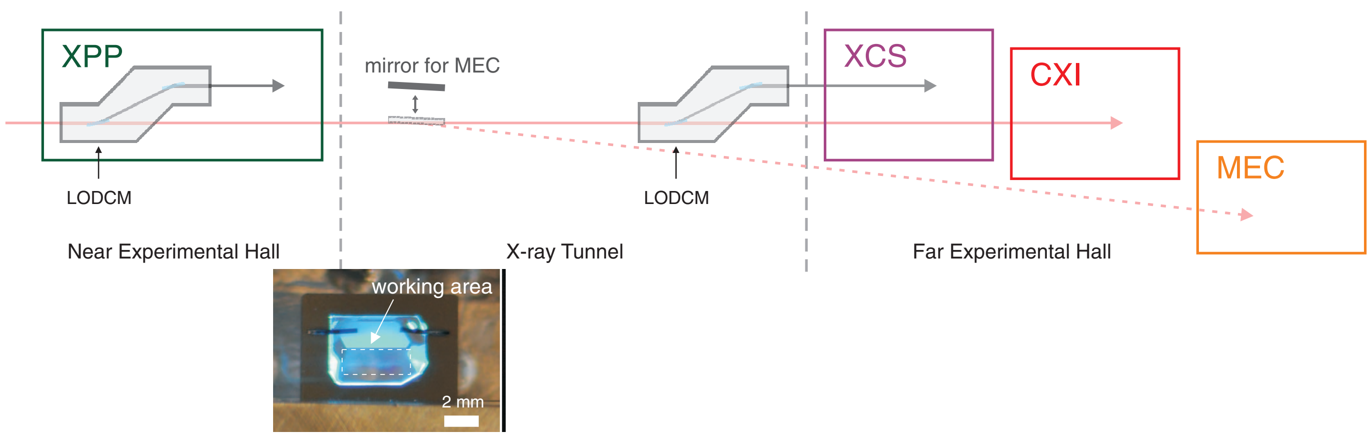


Diamond phase retarder@SACLA



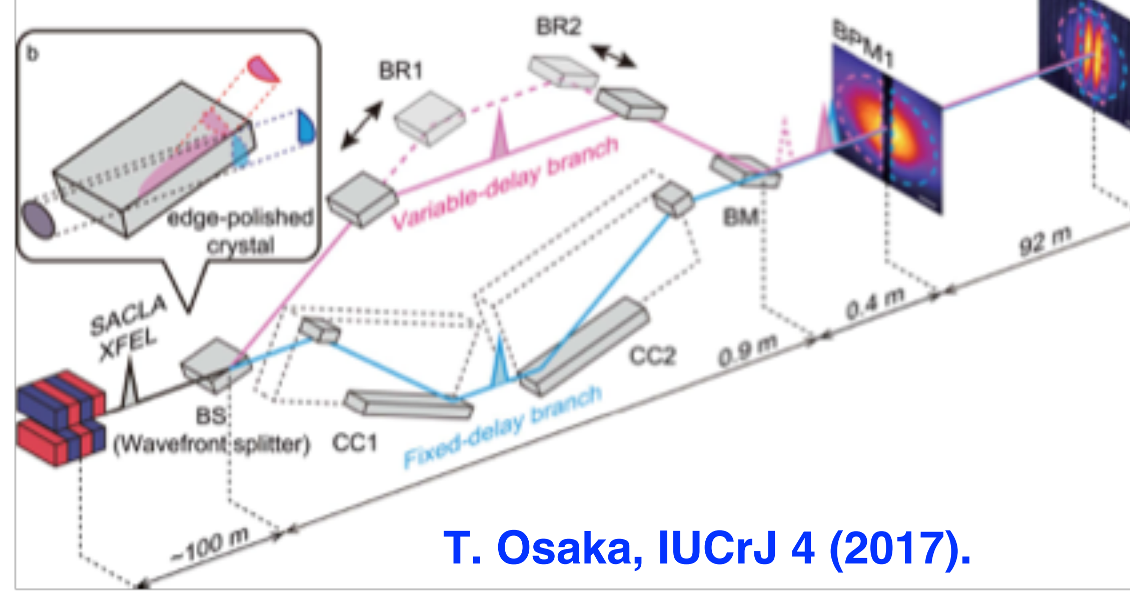
M. Suzuki, JSR 21 (2014).

Large offset diamond monochromator
for beam multiplexing @LCLS



D. Zhu, Rev. Sci. Instrum. 85 (2014).
Y. Feng, Proc. SPIE 8778 (2013).

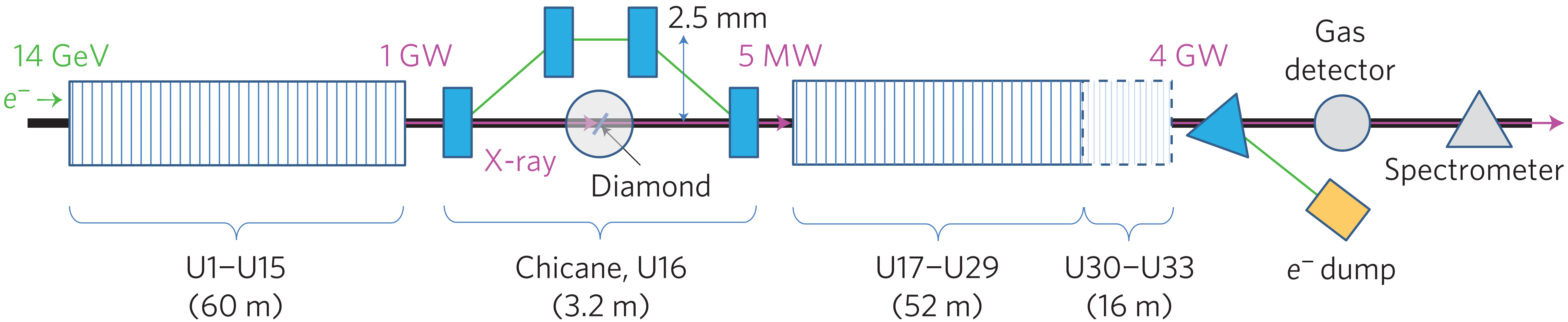
Split-and-delay optics
@SACLA & LCLS

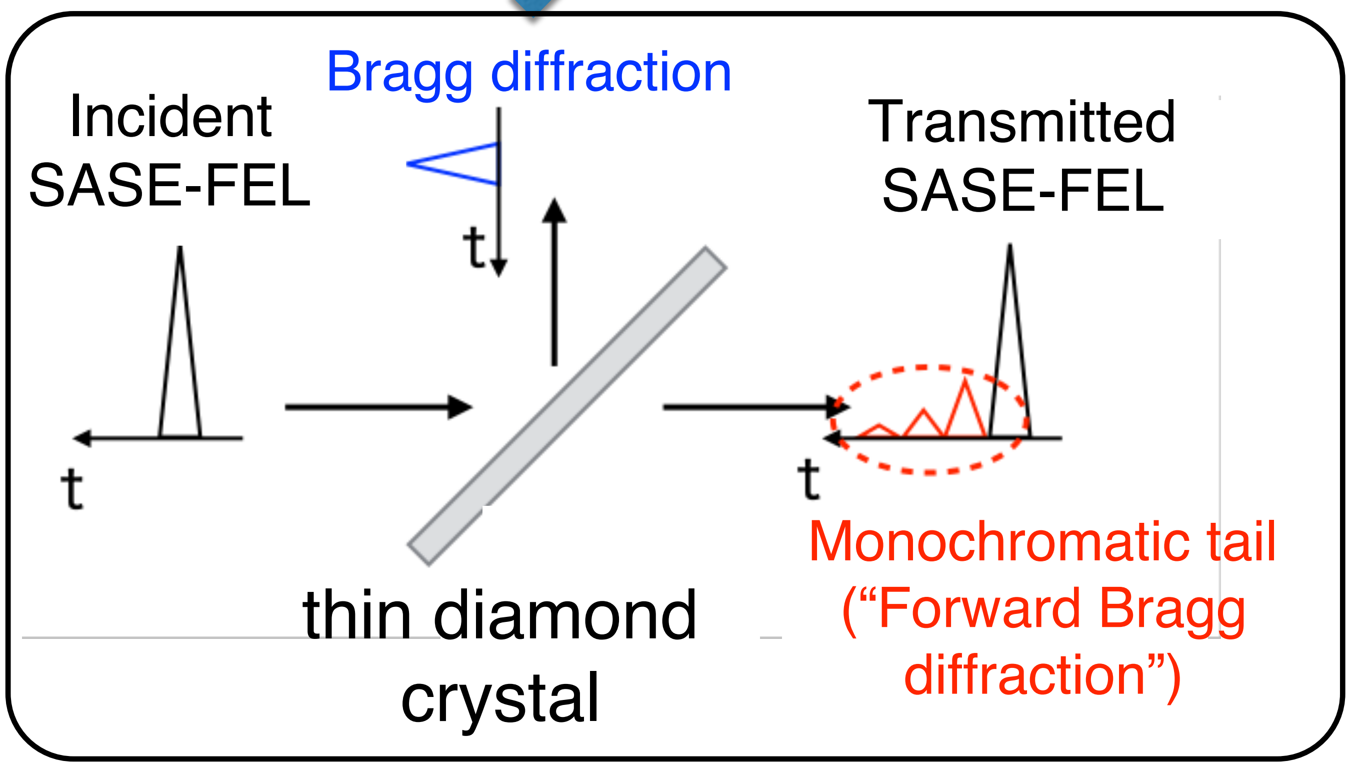


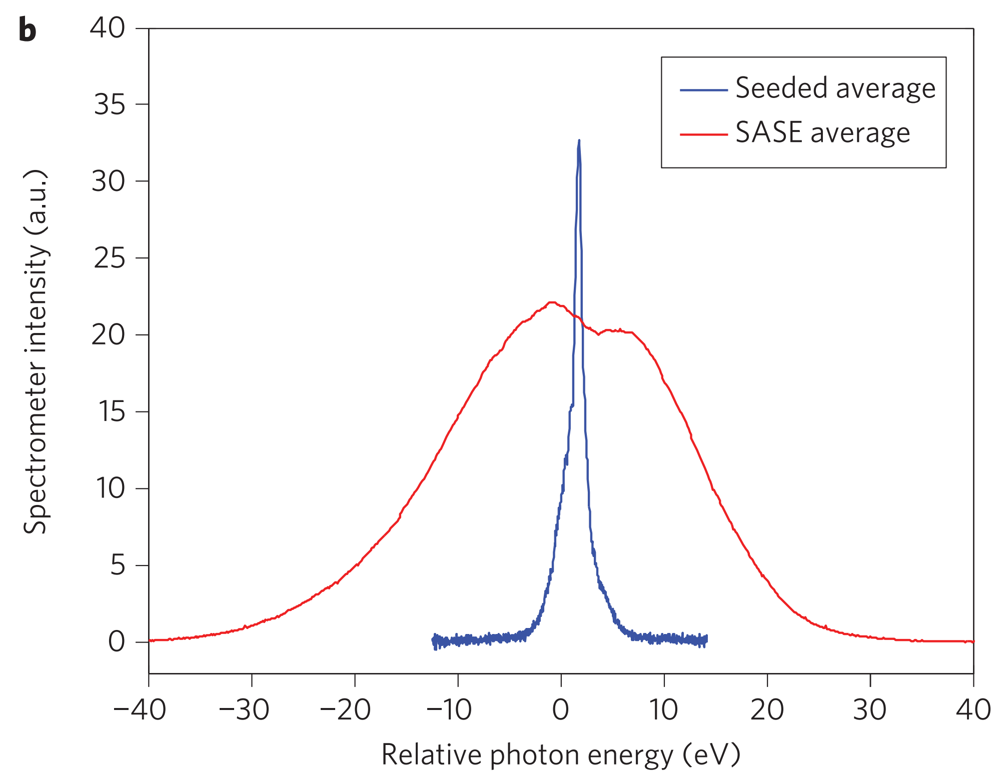
T. Osaka, IUCrJ 4 (2017).

Crystal optics can only reflect X-ray beam with a certain photon energy (The bandwidth of the reflected X-ray beam is a few eV or less): most pulse energy of SASE-XFEL beam is lost in Bragg reflection

Generation of narrow-bandwidth XFELs by self-seeding

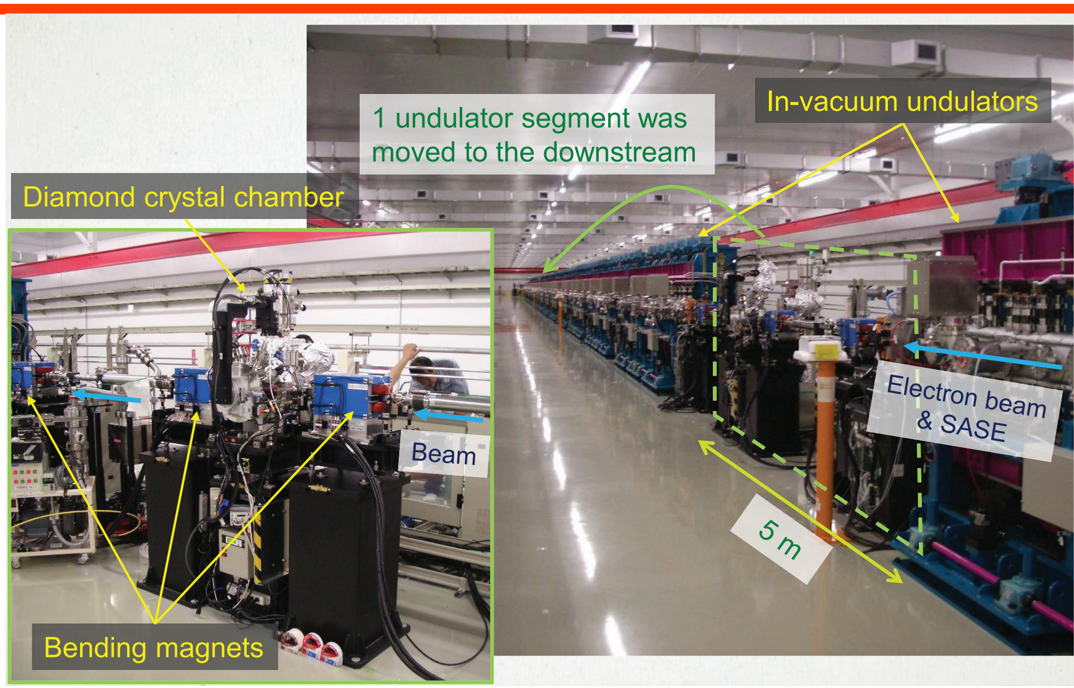


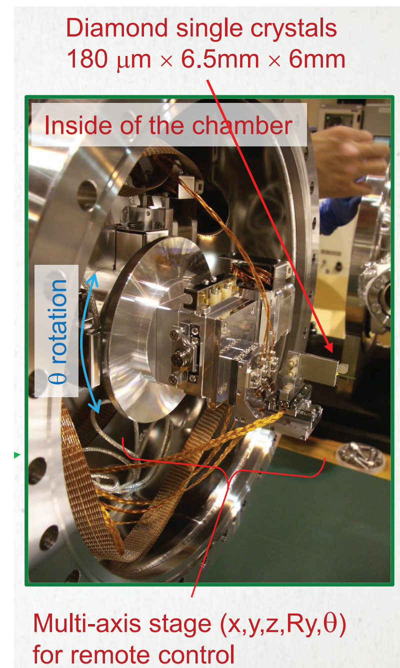


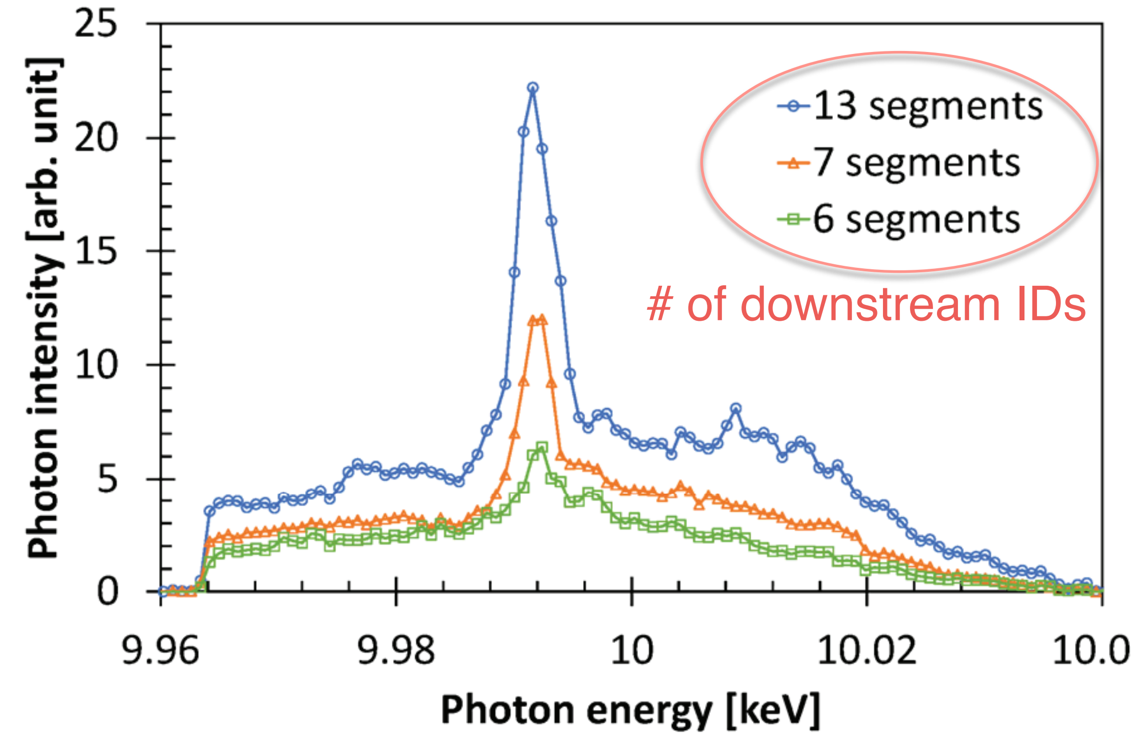


J. Amann *et al.*, *Nat. Photon.* (2012).
R. Lindberg & Yu. Shvyd'ko, *PRST* (2012).

Transmission self-seeding at SACLA BL3







T. Inagaki *et al*., *Proc. FEL 2014*.

Two Problems:

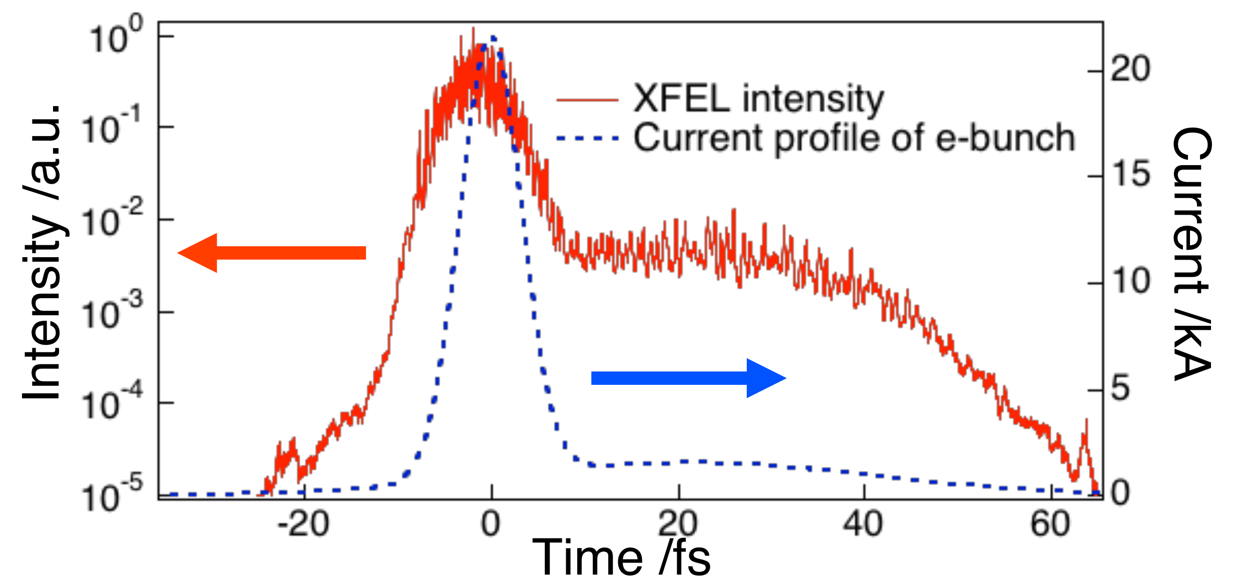
- **Broad SASE background**

→Probably because monochromatic wake and transmitted SASE tail was temporally overlapped and their intensities are comparable

- **Transmitted SASE makes machine tuning difficult**

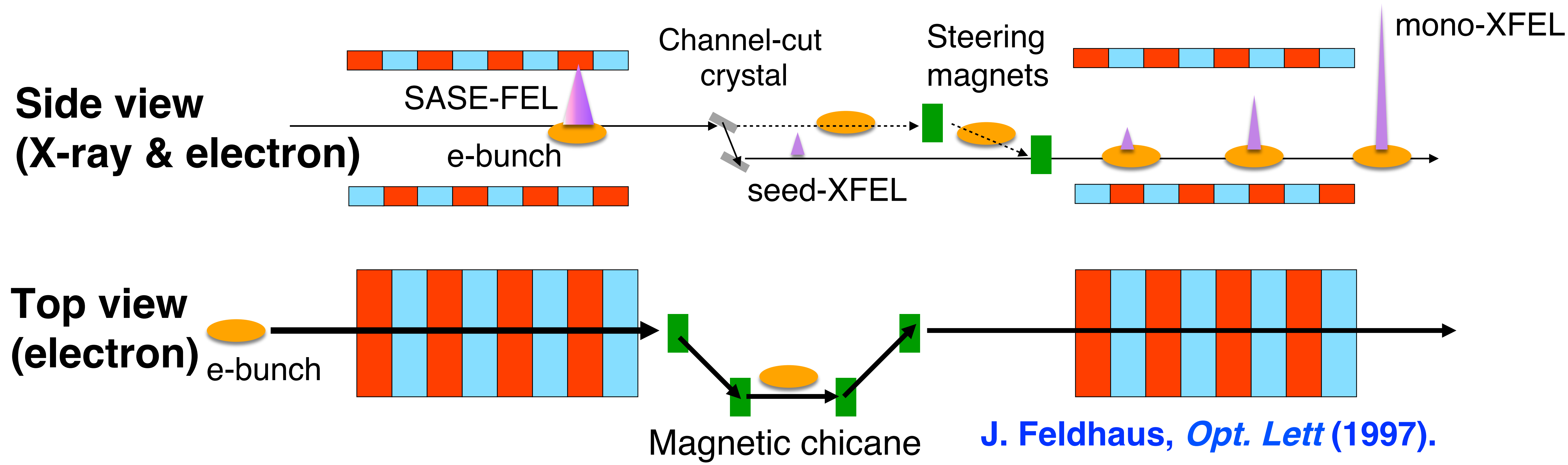
We cannot measure qualities of the seed, such as, intensity, profile, pointing etc.

The e-bunch/XFEL at SACLA has some tails



I. Inoue, *Phys. Rev. Accel. Beams* 21 (2018).

Reflection self-seeding using channel-cut crystal



J. Feldhaus, *Opt. Lett* (1997).

I. Inoue *et al.*, *Nature Photonics* (2019)

☑ Purely mono-XFEL beam is delivered to downstream IDs

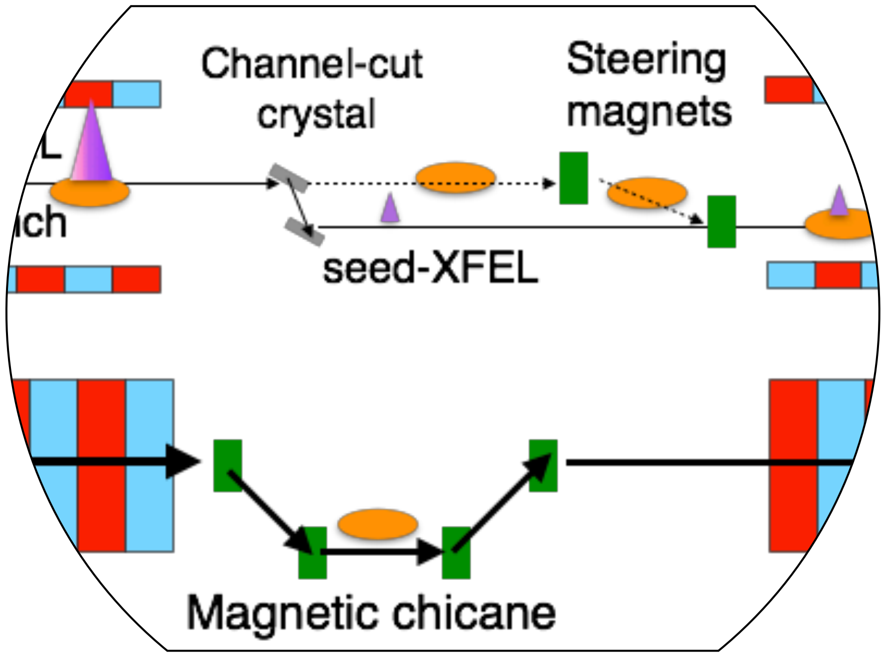
•No SASE contamination in seed pulse

☑ High extraction efficiency of mono-beam from SASE-FEL

$$\frac{\textbf{(Seed power)}}{\textbf{(Input SASE power)}} = \begin{cases} \sim 3\times10^{-2} & \textit{for reflection seeding (Si 111 channel cut)} \\ \sim 5\times10^{-3} \text{ or less} & \textit{for transmission seeding (C400, 100 } \mu m\textit{)} \end{cases}$$

-> seed pulse can be generated with fewer undulators

Difficulty in realizing reflection self-seeding



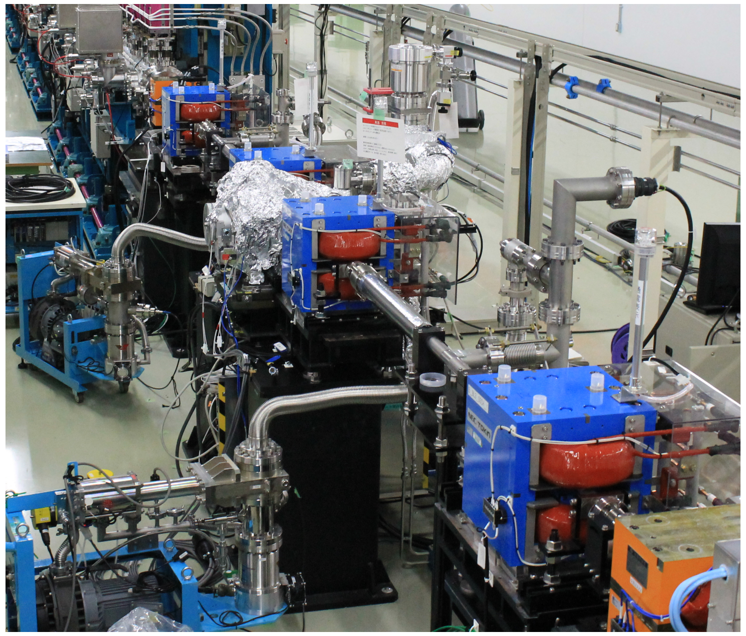
Temporal overlap between seed pulse and e-bunch

(Optical delay by CC-crystal)

|| ~100 ps for typical CC-crystals

(E-bunch delay by magnetic chicane)

Maximum e-bunch delay: ~300 fs

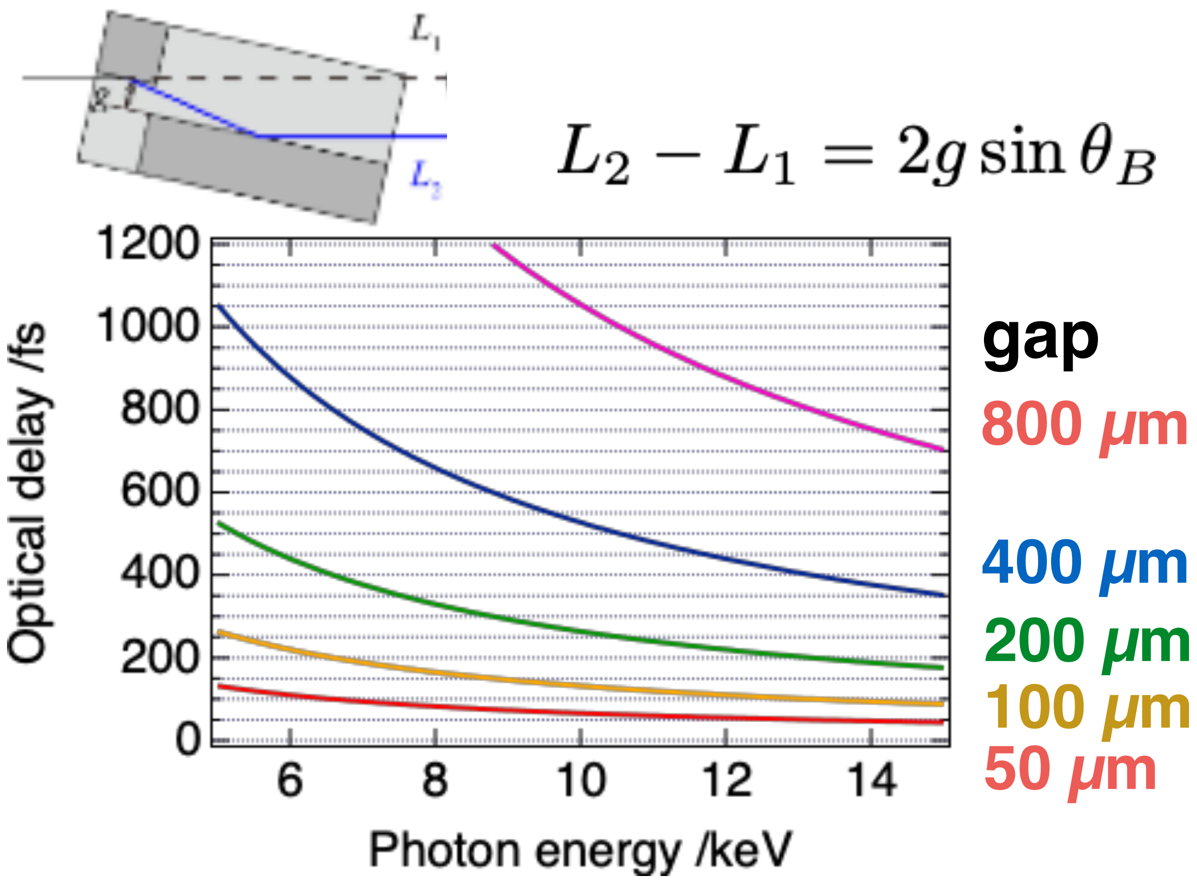


5-m compact chicane enabling large e-beam delay

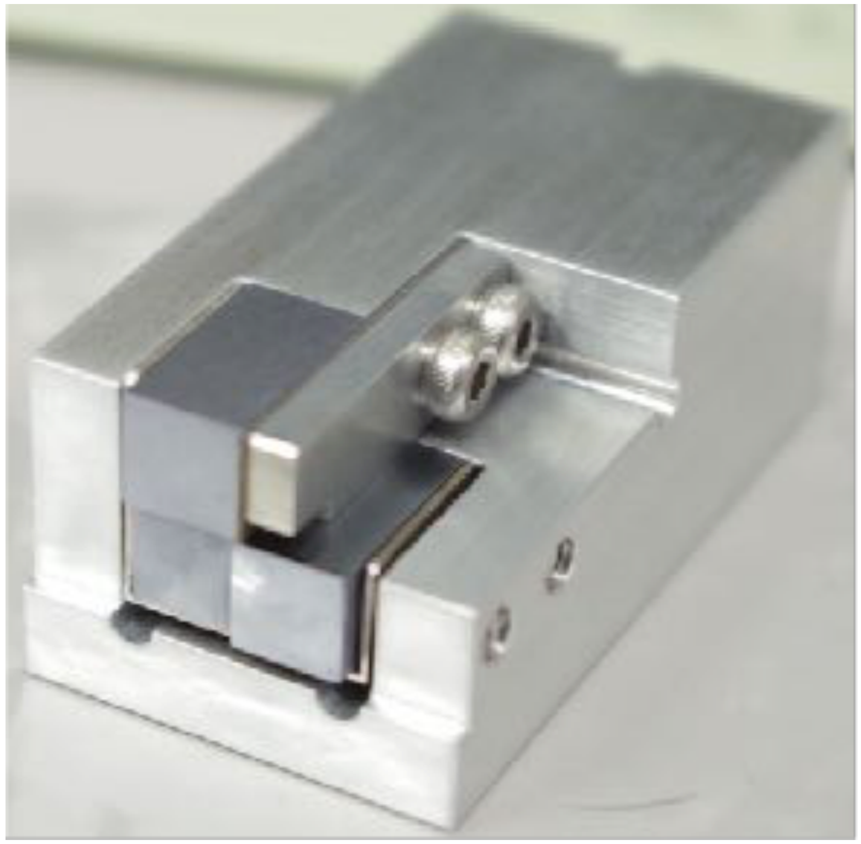
Hara, *Nature Commun.* (2013).
Inoue, *Proc. Natl. Aca. Sci. USA* (2016).

Optical delay by Si 111 CC-crystal

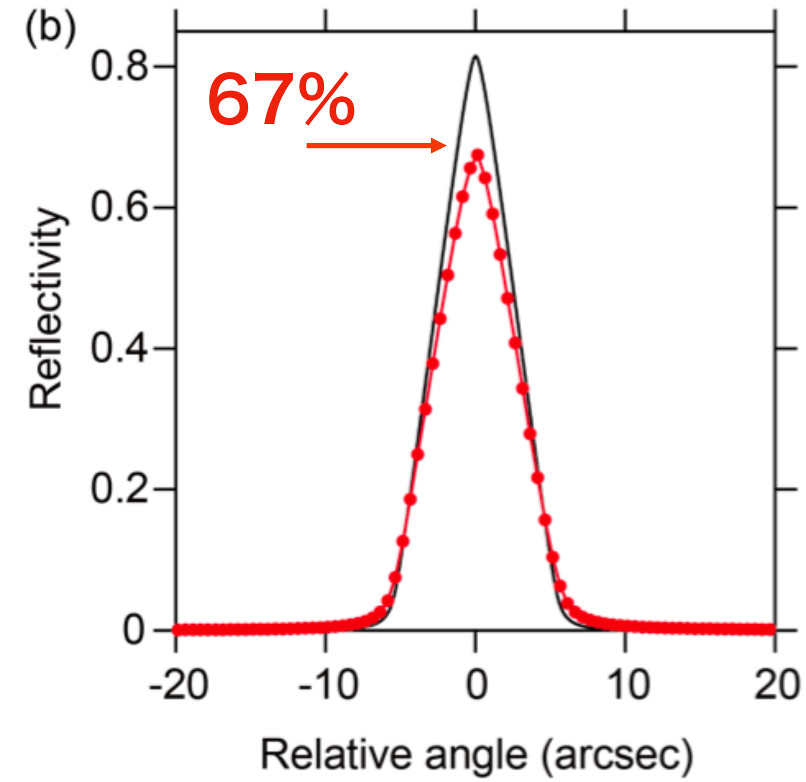
$$L_2 - L_1 = 2g\sin\theta_B$$



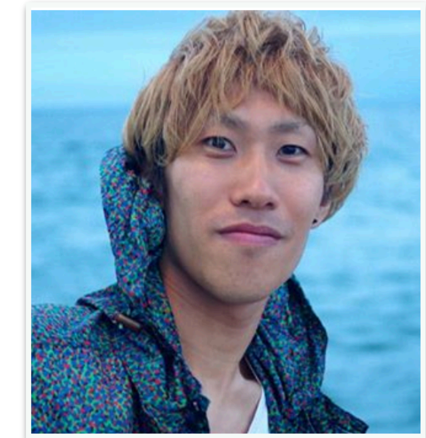
100-μm gap Si(111) channel-cut crystal

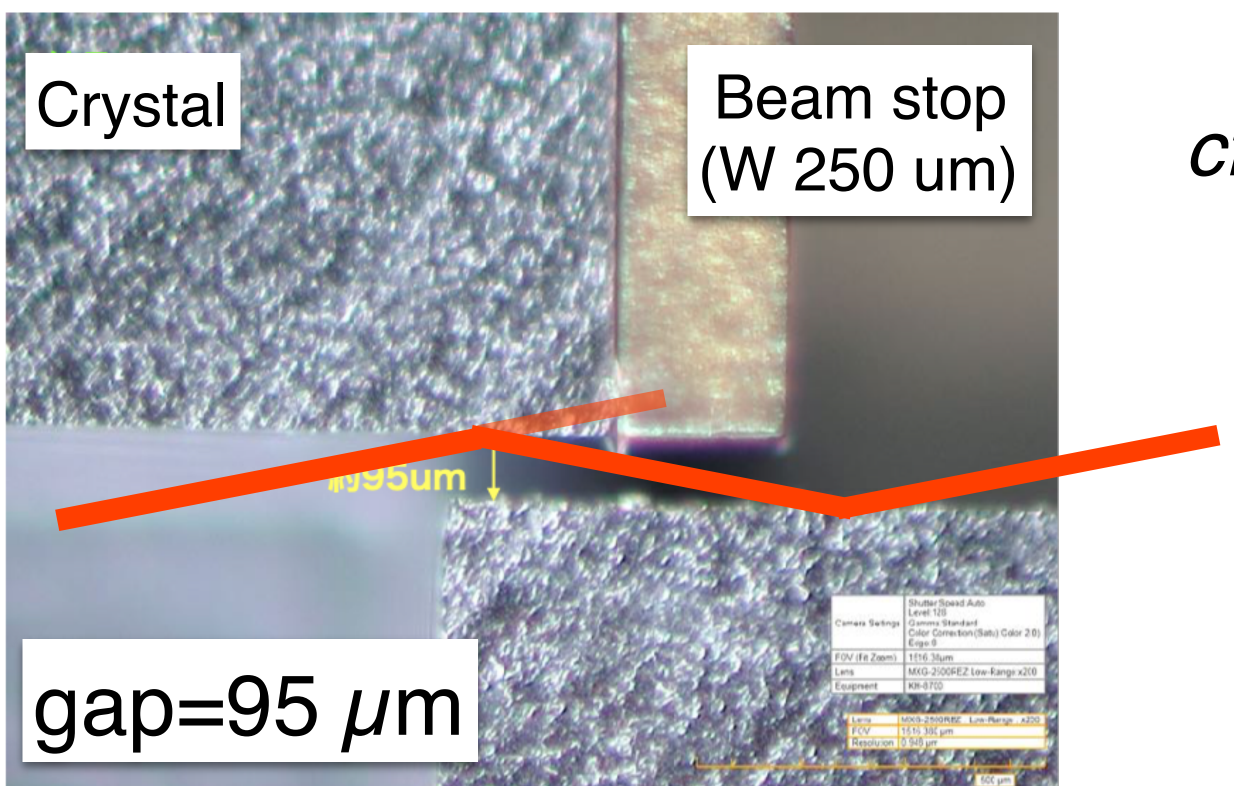


Rocking curve measured with 10-keV SR monochromatized by Si(111) DCM



Taito Osaka
(RIKEN/SACLA)





cf. Theoretical value@peak: ~80%

Photon energy: 5 keV or higher

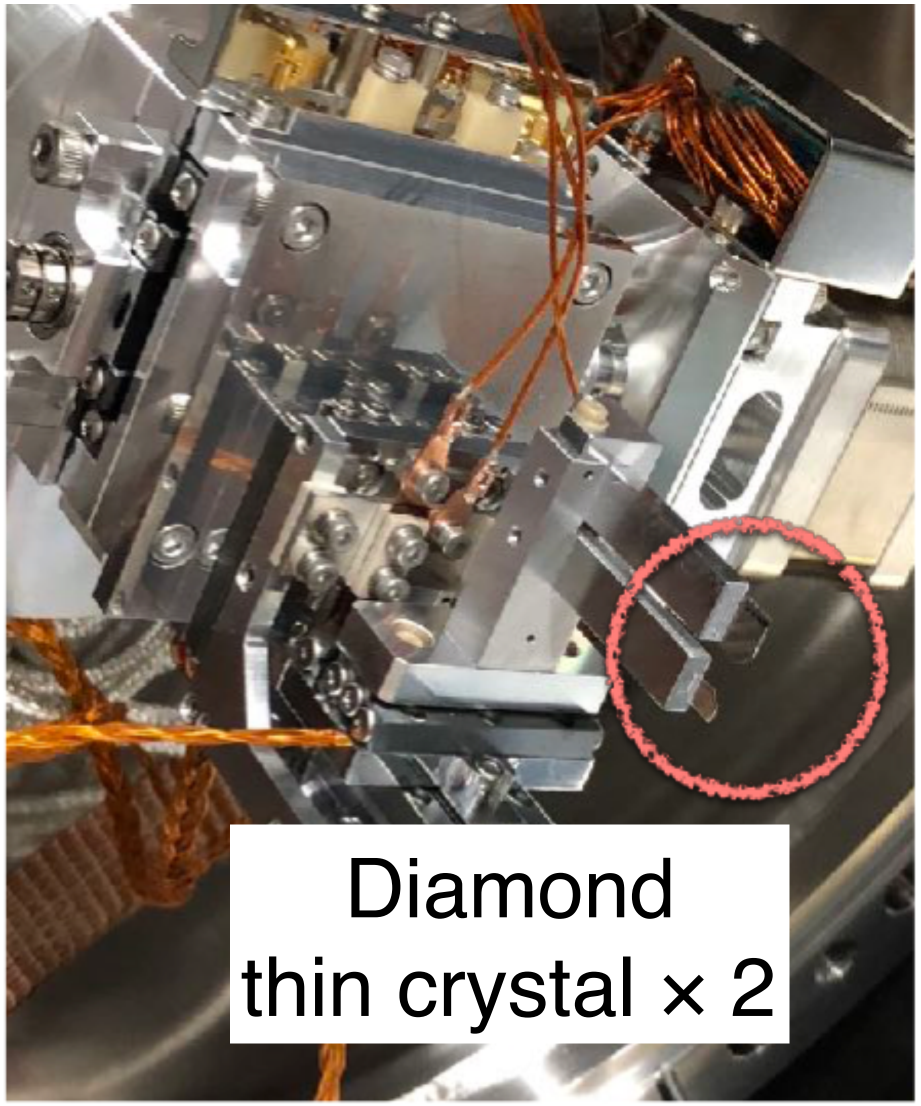
Aperture: 50 μm@10 keV

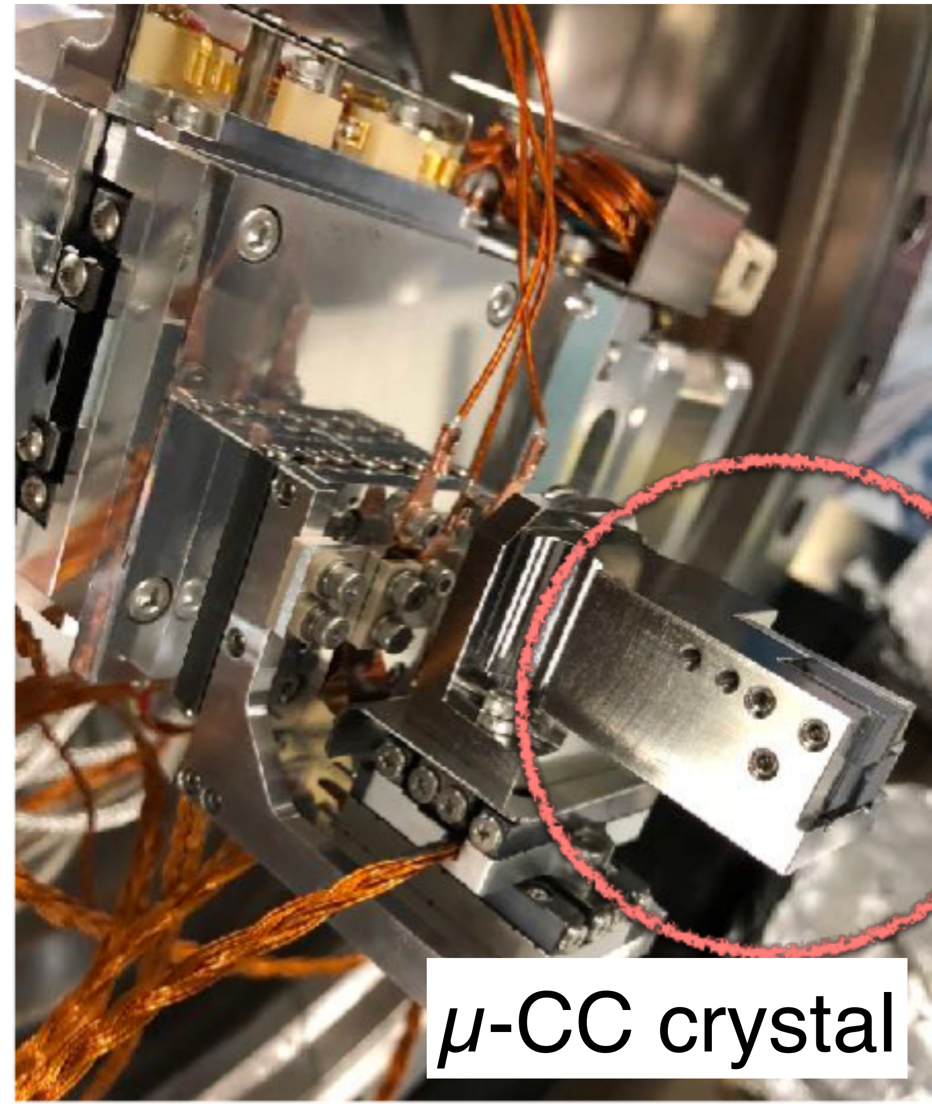
Optical delay: 120 fs@10 keV

X-ray beam offset: 180 μm@10 keV

T. Osaka *et al.*, arXiv: 1811.0860 (2018).

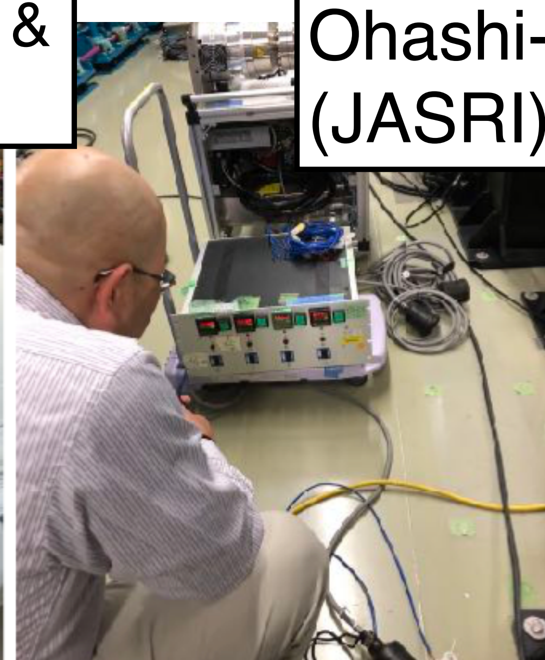
Installation of μ-CC crystal (2017.12.24.)





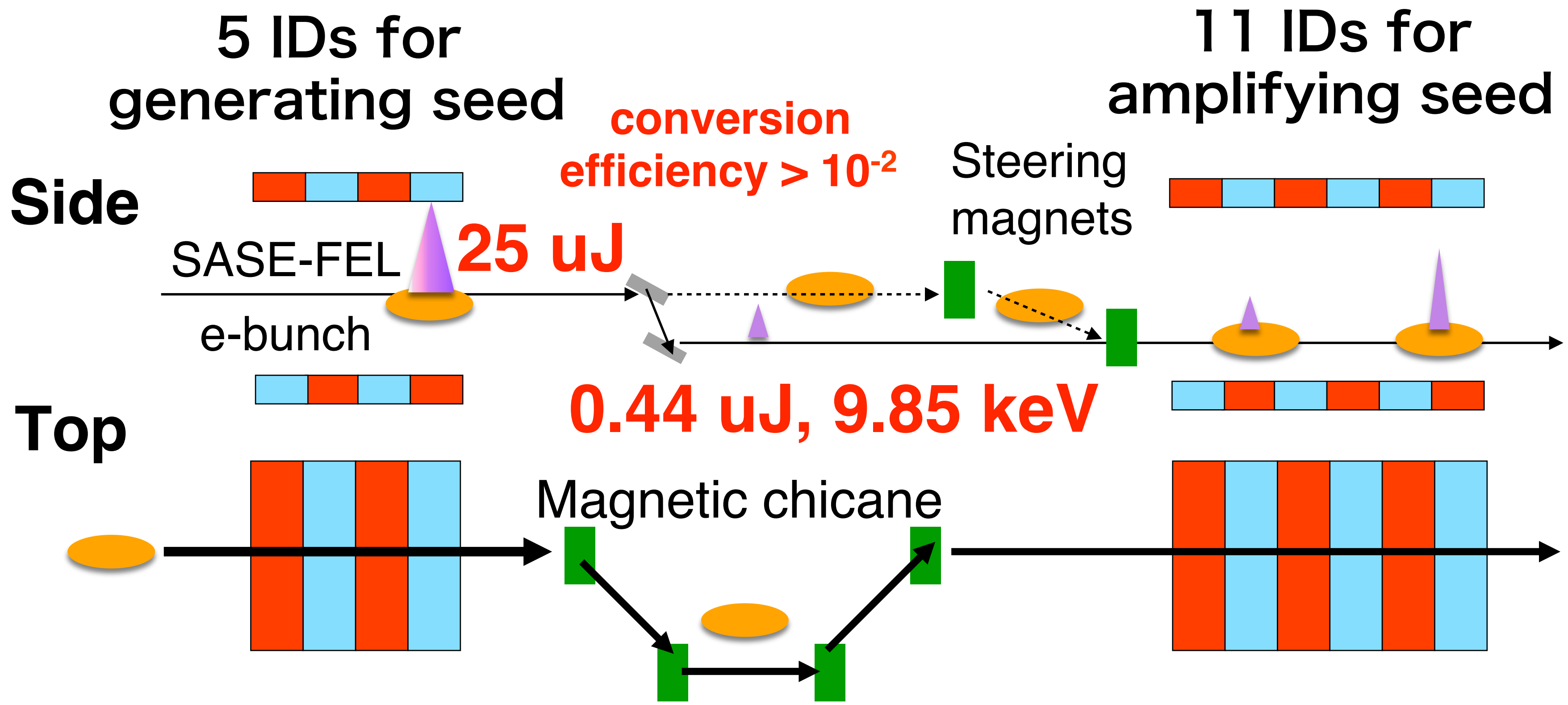
Hasegawa-san (TOYAMA) &
Maki-san (SACLA)

Ohashi-san
(JASRI)

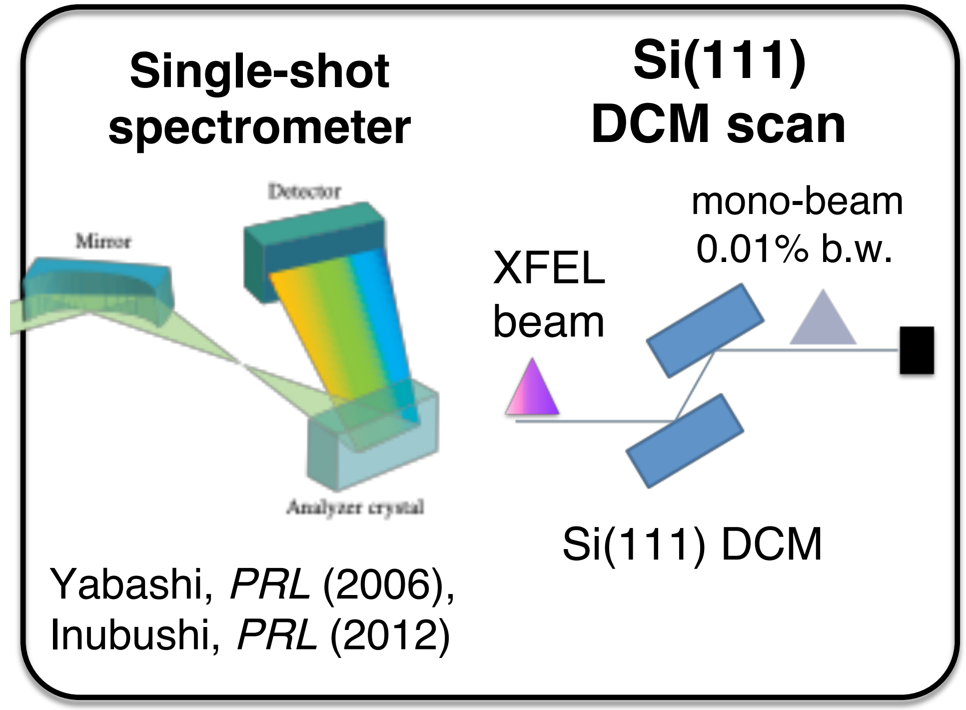


Dec.23-25 2017

Early commissioning results (Jul. 2018)



Photon diagnostics

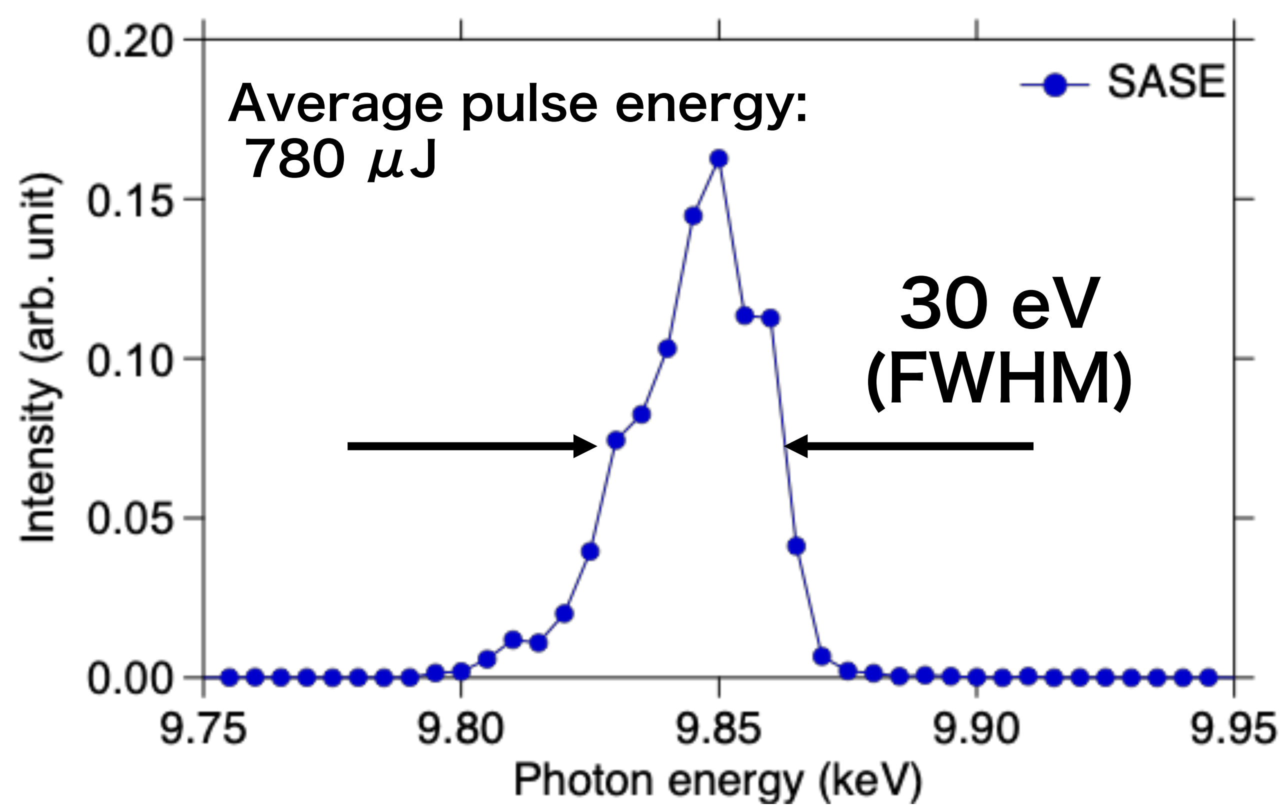


Parameters of e-beam

E-beam energy: 7.8 GeV
E-bunch duration: ~10 fs
E-beam charge: 270 pC
K-value: 2.1
Photon energy: 9.85 keV

The same e-beam parameters for normal SASE mode of SACLA

cf. Average spectrum of SASE-XFEL

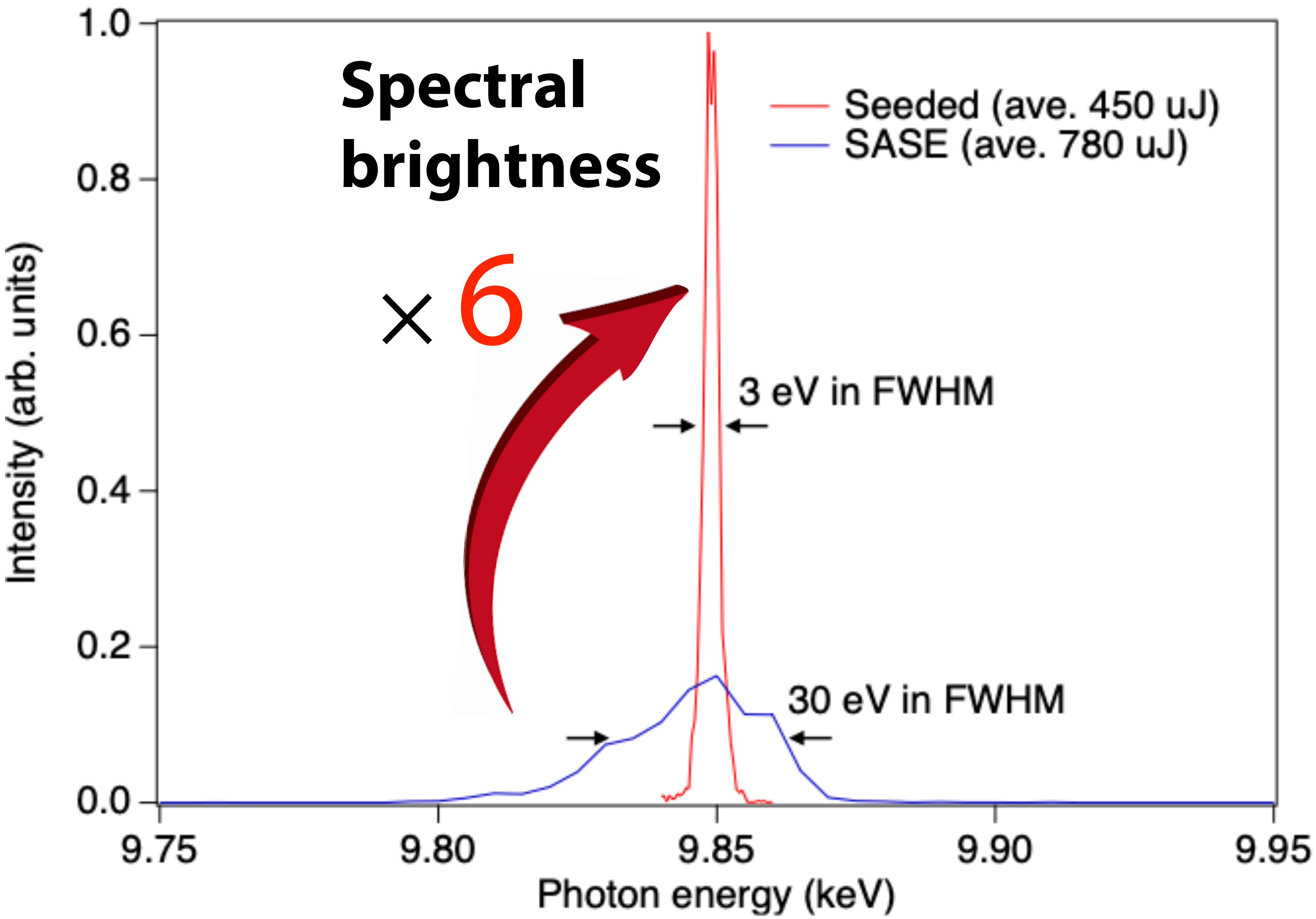


Average spectrum of seeded-XFEL beams

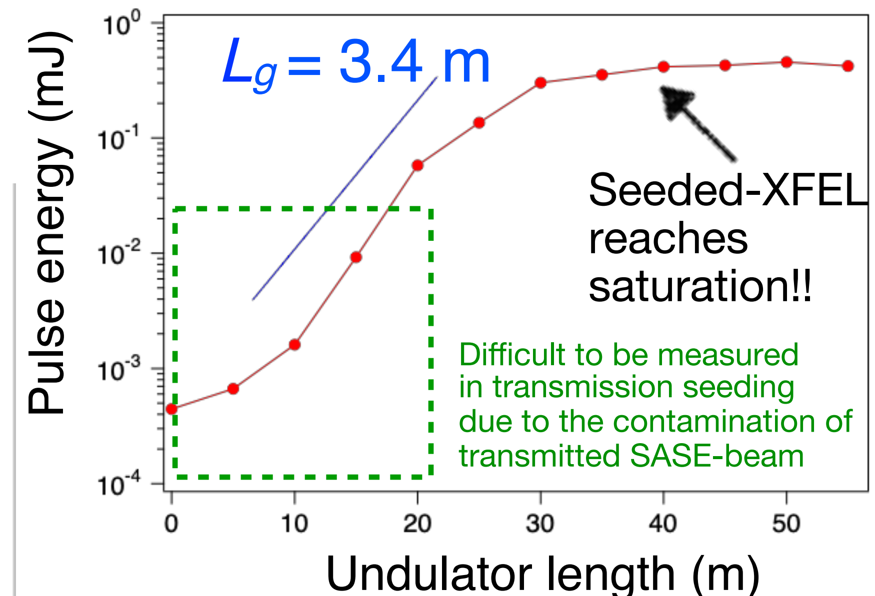
nature photonics
LETTERS
https://doi.org/10.1038/s41566-019-0365-y

Generation of narrow-band X-ray free-electron laser via reflection self-seeding

Ichiro Inoue[1,3*], Taito Osaka[1,3], Toru Hara[1], Takashi Tanaka[1], Takahiro Inagaki[1], Toru Fukui[1], Shunji Goto[1,2], Yuichi Inubushi[1,2], Hiroaki Kimura[1,2], Ryota Kinjo[1], Haruhiko Ohashi[1,2], Kazuaki Togawa[1], Kensuke Tono[1,2], Mitsuhiro Yamaga[1,2], Hitoshi Tanaka[1], Tetsuya Ishikawa[1] and Makina Yabashi[1,2]



Gain curve of seeded-XFEL beam

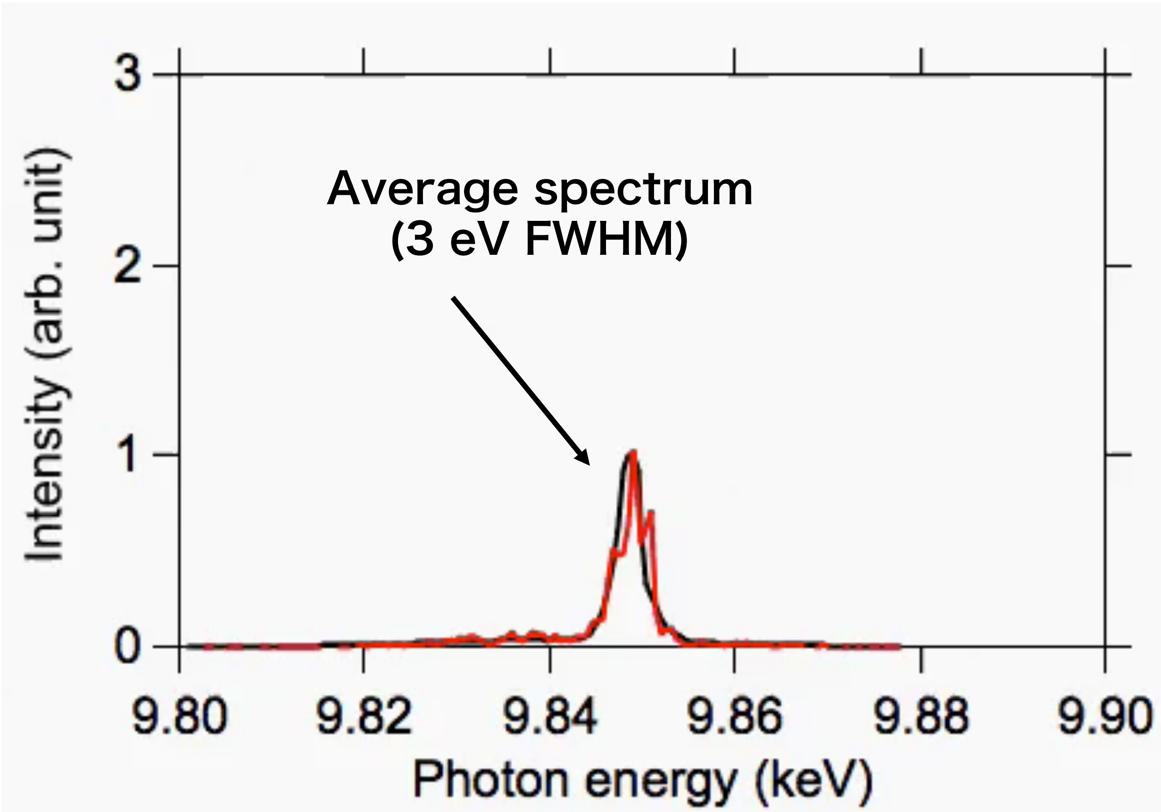


☑ Intensity gain length ($L_g = 3.4$ m) was comparable to that of normal SASE mode ($L_g = 2.3$ m).

→Degradation of electron beam quality caused by XFEL amplification at upstream IDs was not severe.

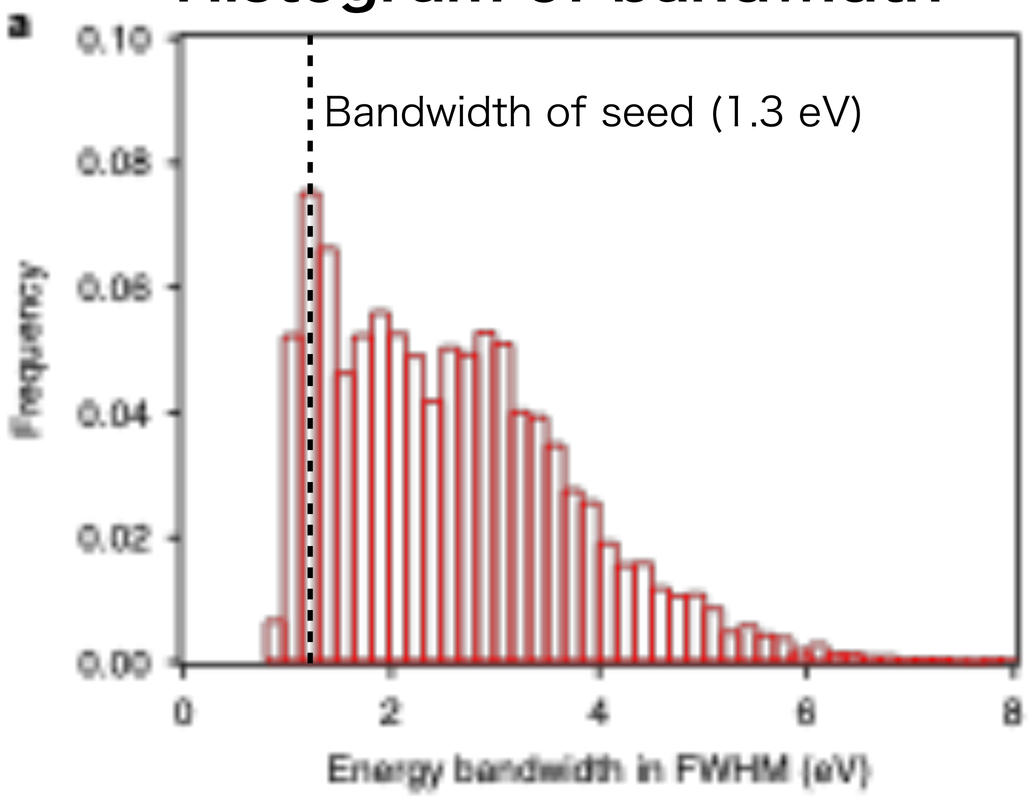
I. Inoue *et al.*, *Nature Photon.* (2019).

Single-shot spectrum of seeded-XFEL beam

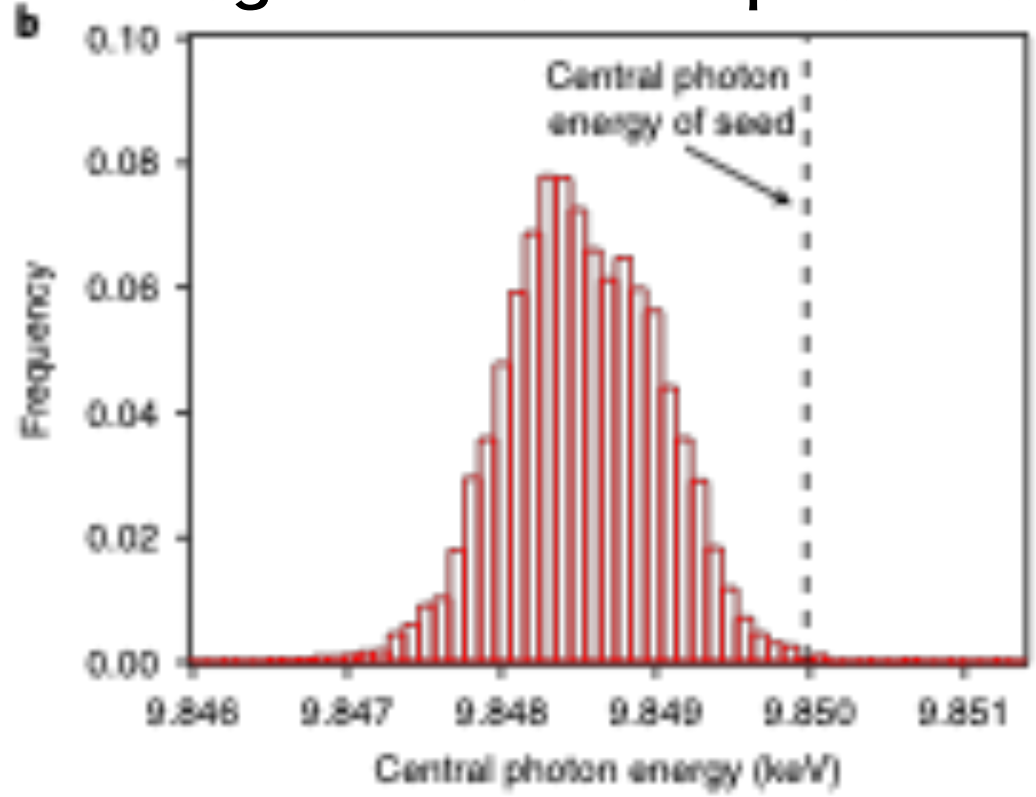


- ☑ Central photon energy of seeded-XFEL is slightly lower than that of seed
- ☑ Bandwidth of seeded-XFEL is larger than that of seed

Histogram of bandwidth

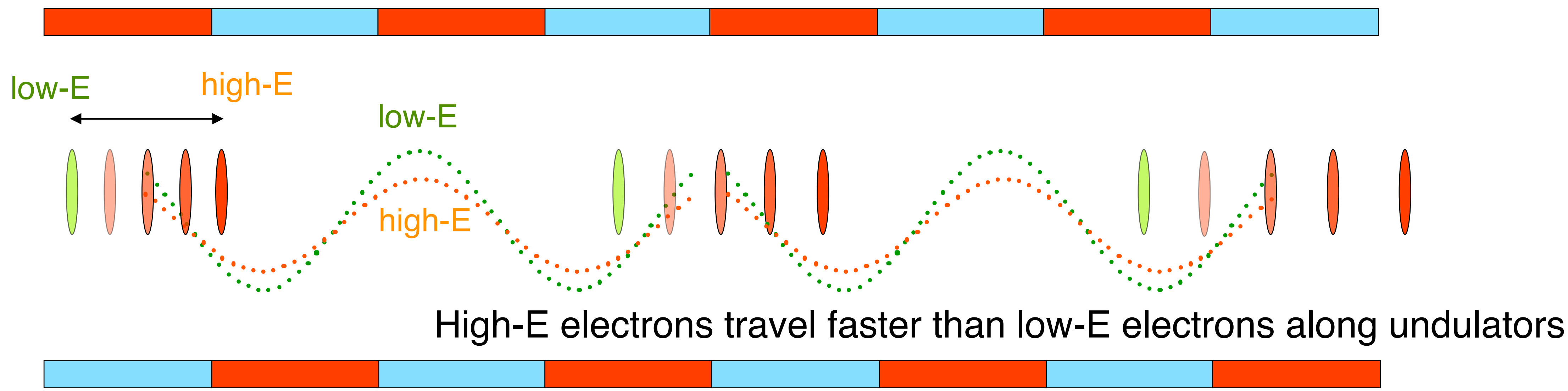


Histogram of central photon energy



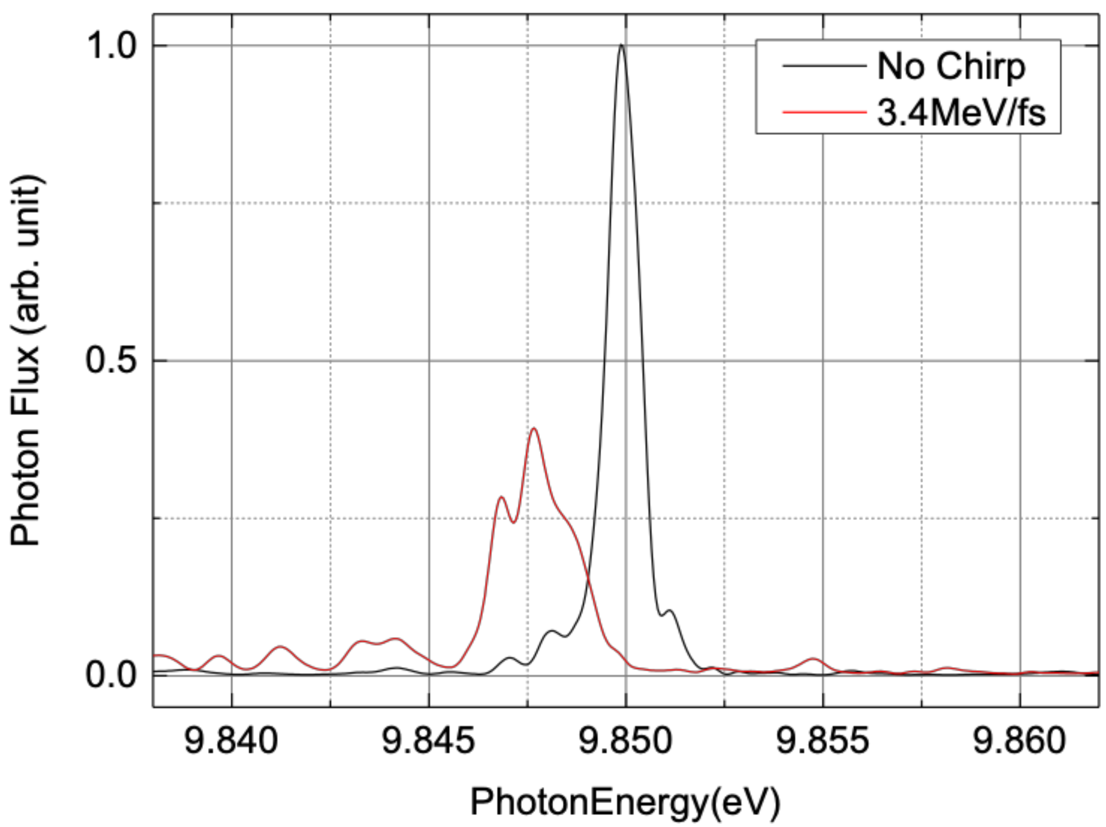
I. Inoue *et al., Nature Photon.* (2019).

Effect of energy chirp on the spectrum



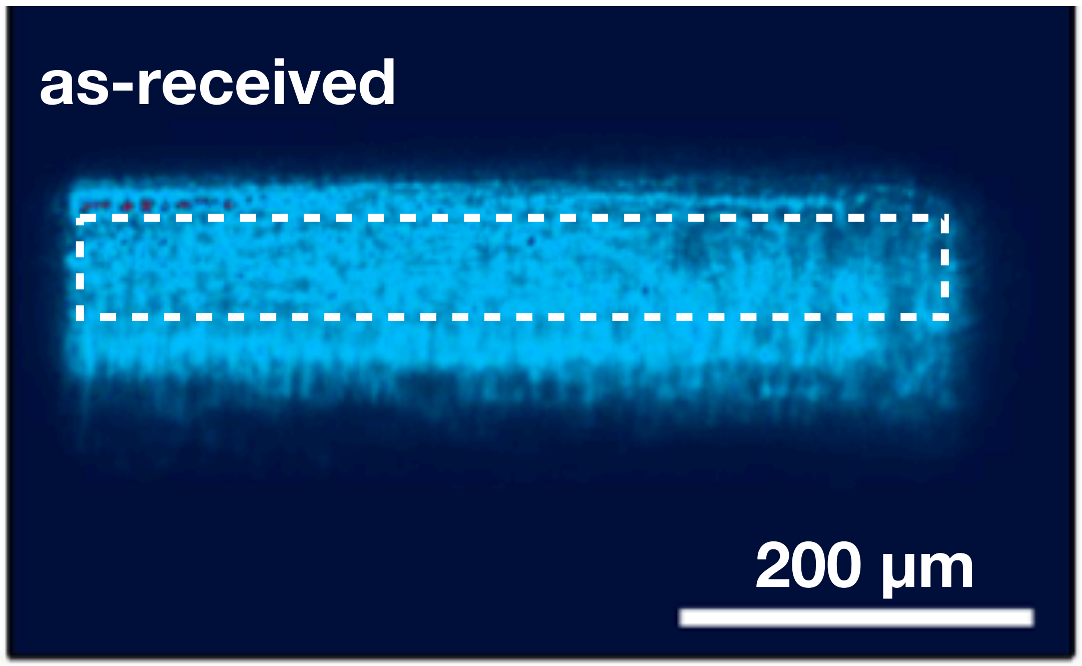
If there is non-negligible energy chirp of e-beam,
intervals of micro-bunches gradually changes along the undulators.

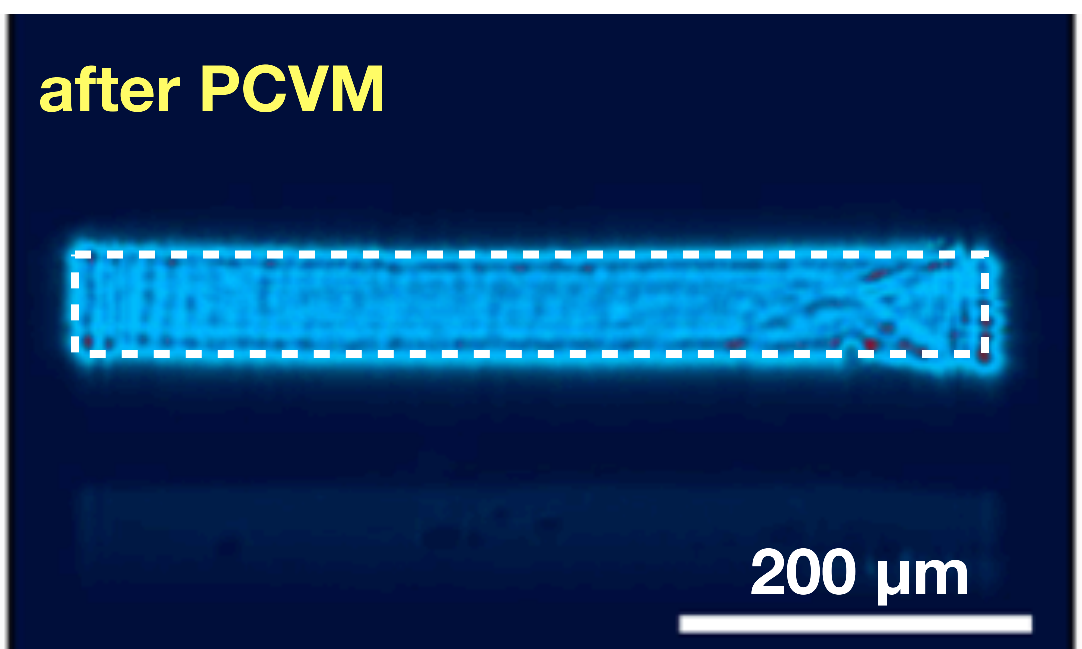
e.g.
FEL simulation of seeded-XFELs with/without energy chirp of e-beam



Towards narrower and brighter seeded-XFELs

- ☐ smaller energy chirp in the e⁻ beam → difficult to be realized immediately
- ☑ narrower bandwidth of the seed → use of higher order diffraction (Si 220)



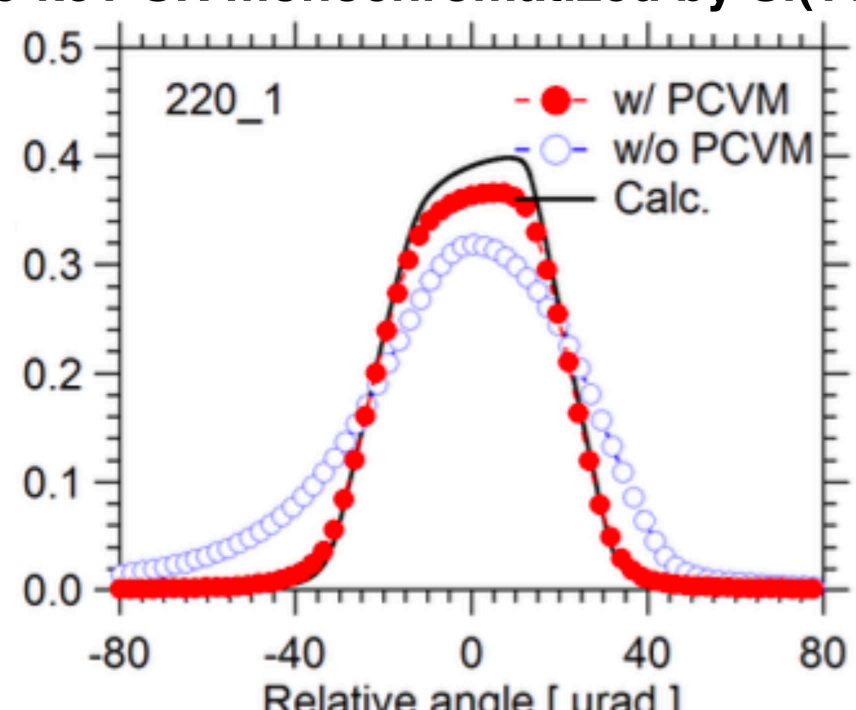


Diffraction in higher order indices is more sensitive to lattice strain.
much distorted wavefront

T. Hirano (Osaka U) treated the Si(220) crystal with a plasma etching technique (**PCVM**).

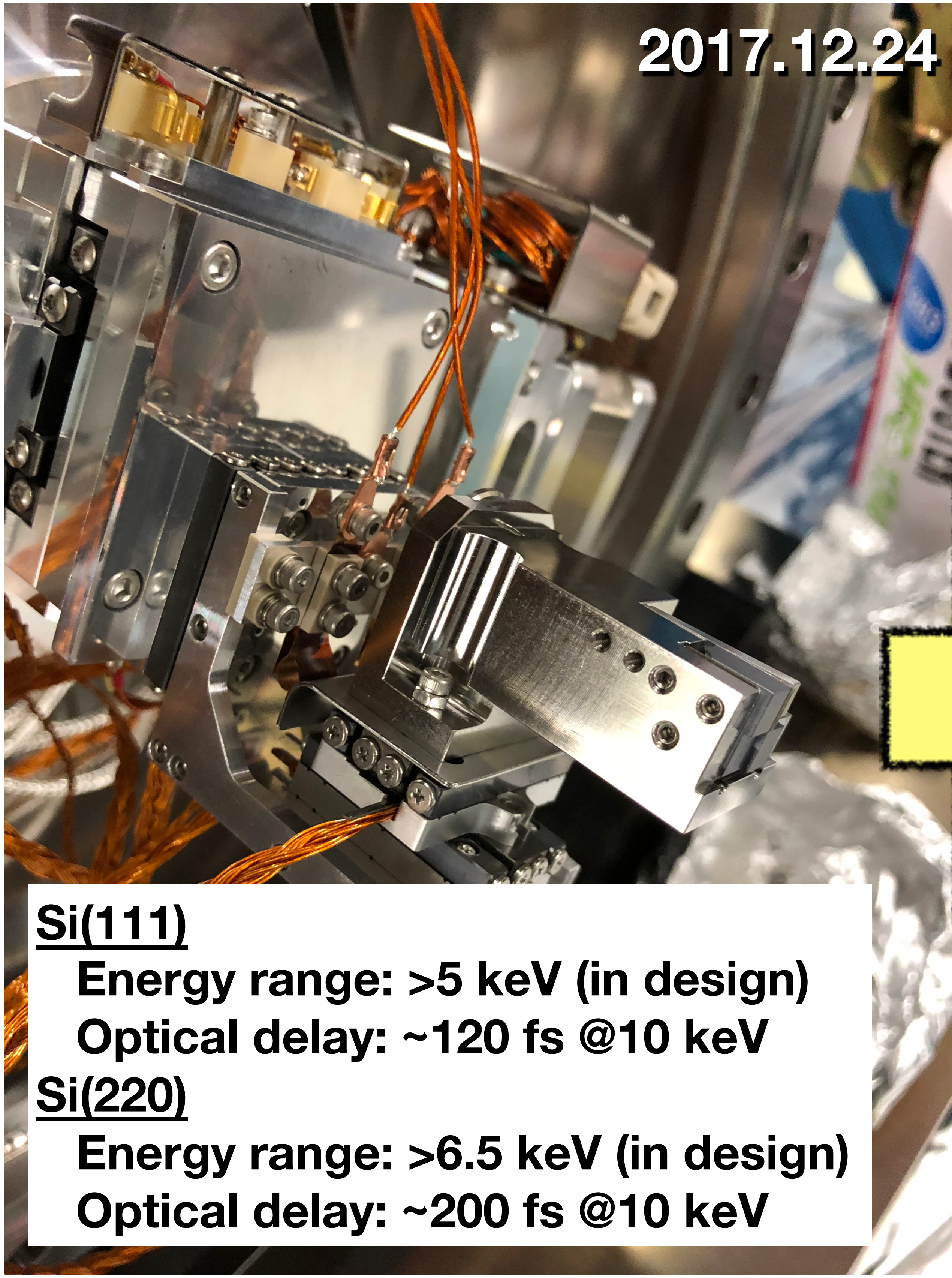
Nearly ideal reflection profile & rocking curve

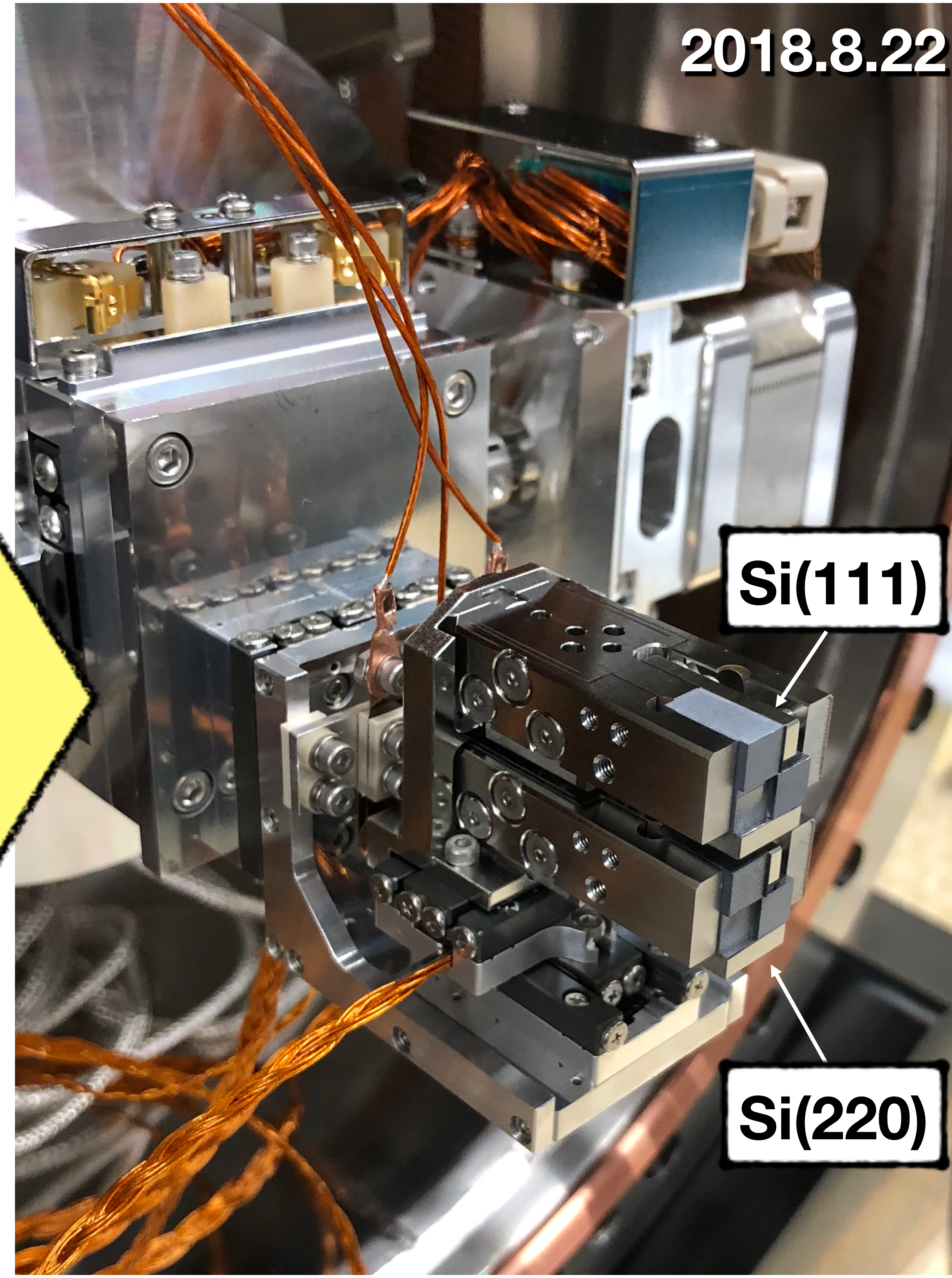
Rocking curve measured with 10-keV SR monochromatized by Si(111) DCM



Takashi Hirano (Osaka U)

Installation of Si(220) crystal (2018.8.22.)





<u>Si(111)</u>
Energy range: >5 keV (in design)
Optical delay: ~120 fs @10 keV

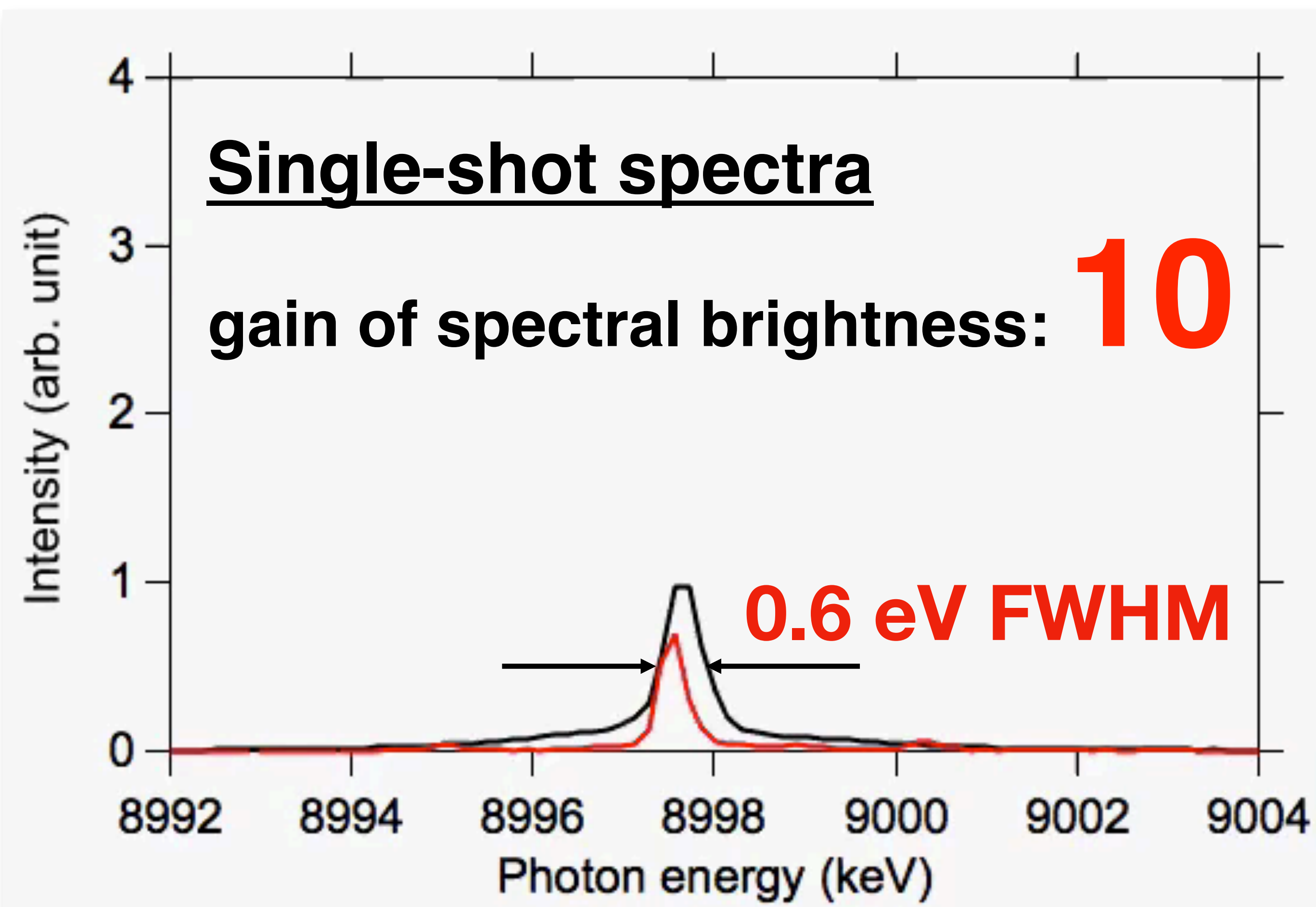
<u>Si(220)</u>
Energy range: >6.5 keV (in design)
Optical delay: ~200 fs @10 keV

Seeded-XFELs generated with Si (220) crystal

Typical gain of spectral brightness by Si (220) seeding with respect to normal SASE mode is ~7

cf. typical gain with Si (111) seeding: ~6

If the electron beam condition is good
(unfortunately we cannot routinely achieved this good condition),
the bandwidth of seeded-XFEL and seed becomes almost the same



Osaka *et al., in preparation.*

Average bandwidth (0.6 eV) is almost the same as that of the seed (0.5 eV).

cf.
XFEL pulse duration of SACLA is 6 fs
→Seeded-XFEL is nearly Fourier-transform-limited.

Early user experiments (since June 2018, # of experiments: 8)

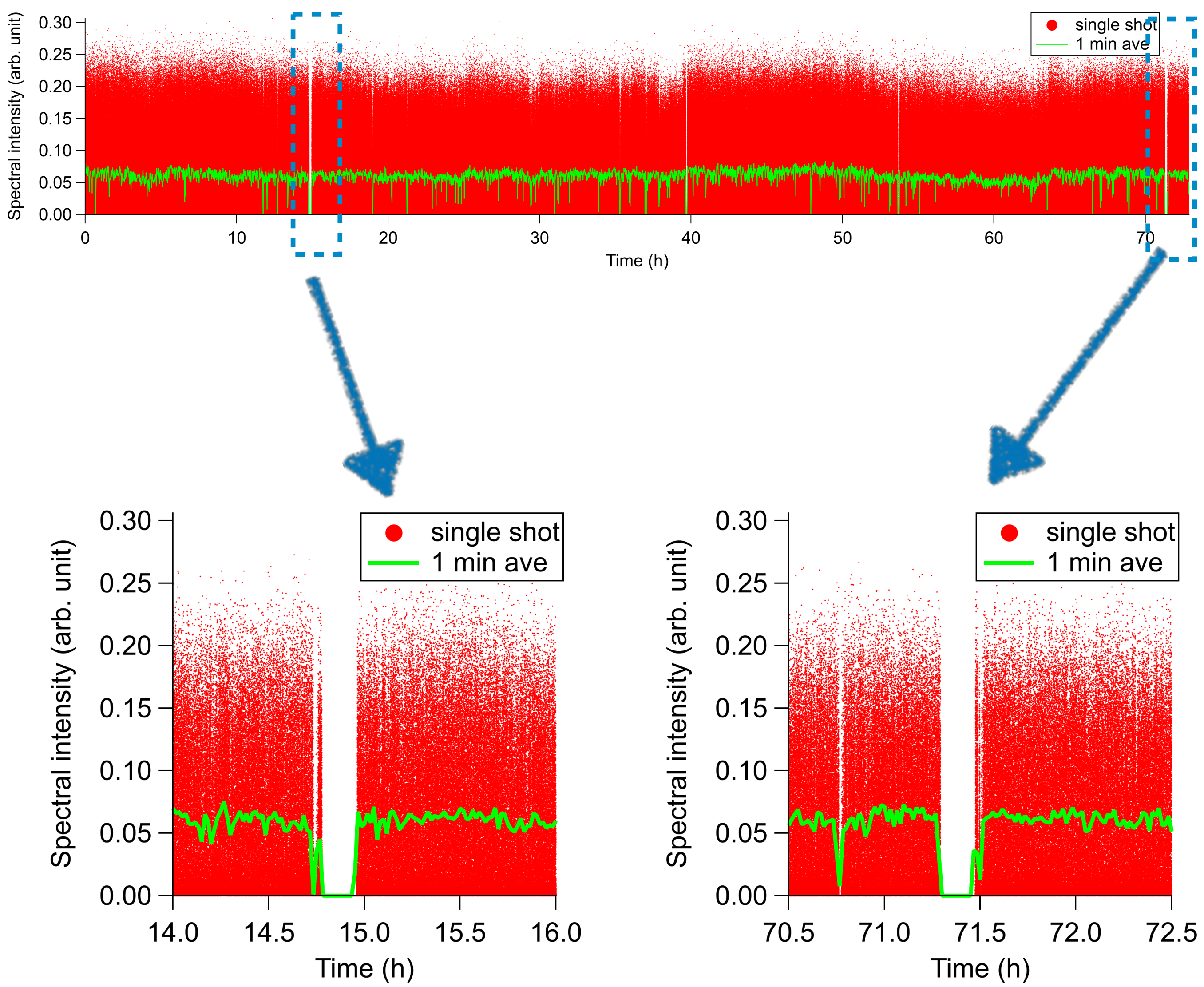
Typical tuning time

1. Tune normal SASE with full IDs including spectrum & optical axis **~2 h**
2. Open the downstream IDs & adjust μCC **1~2 h**
3. Close the downstream IDs & adjust the optical axis **~0.5 h**
4. Set delay and offset for e– beam to calculated values, then adjust the optical axis of SASE to the seed position **~0.5 h**
5. Optimize some parameters of the downstream IDs by monitoring pulse energies after the Si(111) DCM (e– beam offset both in Ver. & Hor., K value, taper of IDs, delay etc.) **3~4 h**

Just realizing seeded-XFEL: ~4 hours
Optimizing seeding conditions: ~8 hours
Not short but straightforward.
(All processes can be completed by Accel. operators without help of scientists)

Long term stability

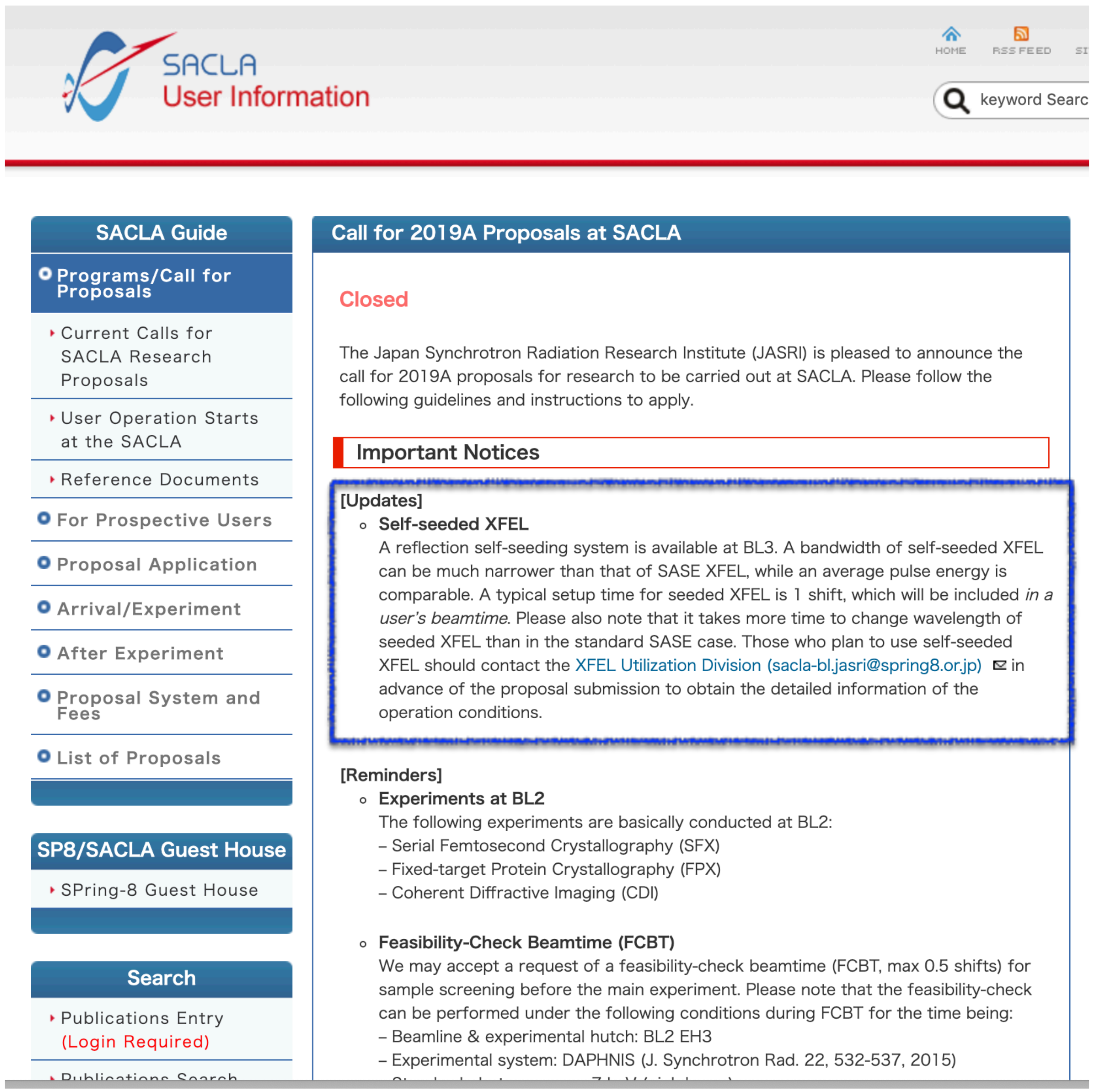
XFEL intensity after Si (111)DCM @ User experiments(Dec. 2018)



Spectral brightness kept its original value over 3 days (=typical beam time for single user)

Self-seeding is officially released for user experiments

From the current run (2019A: Apr.-Aug. 2019),
seeded-XFEL is released for user experiments as a standard operat



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Call for 2019A Proposals at SACLA

Closed

The Japan Synchrotron Radiation Research Institute (JASRI) is pleased to announce the call for 2019A proposals for research to be carried out at SACLA. Please follow the following guidelines and instructions to apply.

Important Notices

[Updates]

- **Self-seeded XFEL**
  A reflection self-seeding system is available at BL3. A bandwidth of self-seeded XFEL can be much narrower than that of SASE XFEL, while an average pulse energy is comparable. A typical setup time for seeded XFEL is 1 shift, which will be included *in a user's beamtime*. Please also note that it takes more time to change wavelength of seeded XFEL than in the standard SASE case. Those who plan to use self-seeded XFEL should contact the XFEL Utilization Division (sacla-bl.jasri@spring8.or.jp) in advance of the proposal submission to obtain the detailed information of the operation conditions.

[Reminders]

- **Experiments at BL2**
  The following experiments are basically conducted at BL2:
  – Serial Femtosecond Crystallography (SFX)
  – Fixed-target Protein Crystallography (FPX)
  – Coherent Diffractive Imaging (CDI)
- **Feasibility-Check Beamtime (FCBT)**
  We may accept a request of a feasibility-check beamtime (FCBT, max 0.5 shifts) for sample screening before the main experiment. Please note that the feasibility-check can be performed under the following conditions during FCBT for the time being:
  – Beamline & experimental hutch: BL2 EH3
  – Experimental system: DAPHNIS (J. Synchrotron Rad. 22, 532-537, 2015)

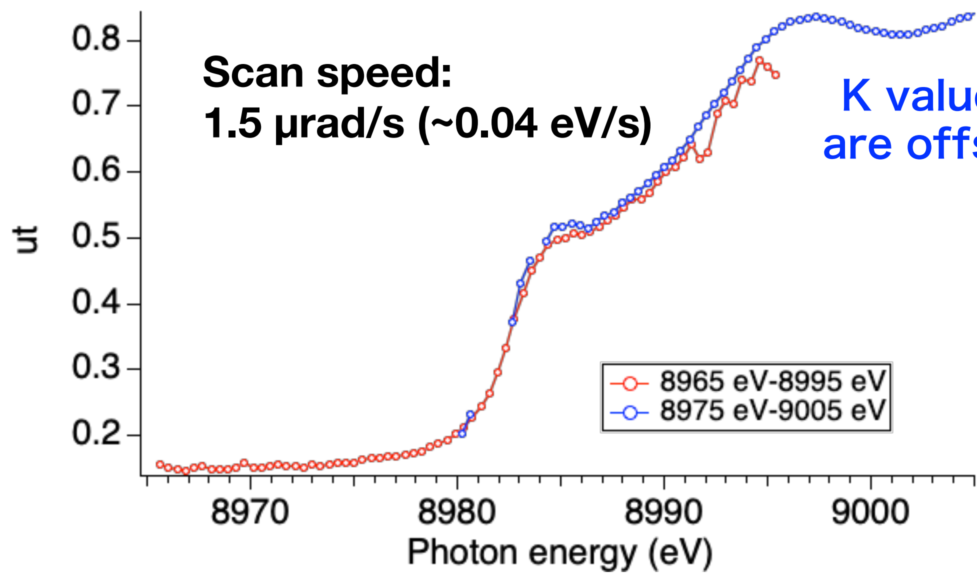
Homepage of call for 2019A Proposals at SACLA

~25% of all scheduled experiments at SACLA BL3 will utilize seeded-XFEL beam

On-going projects

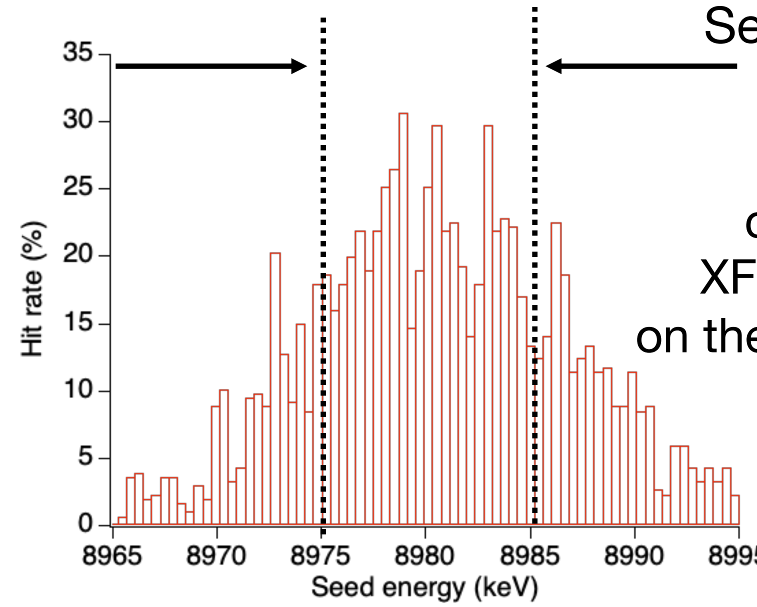
☑Fast photon energy scan (continuously rotating seed Xtal)

XANES spectrum of Cu 10 um



K values of all IDs are offset by +5 eV

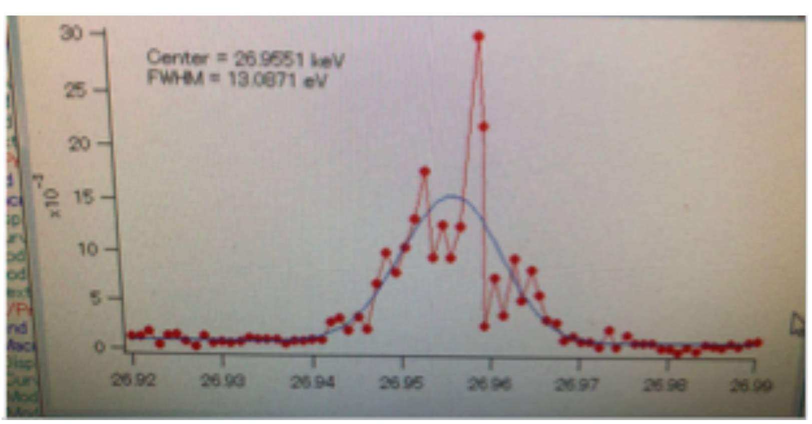
Proportion of intense and narrowband seeded-XFEL pulses



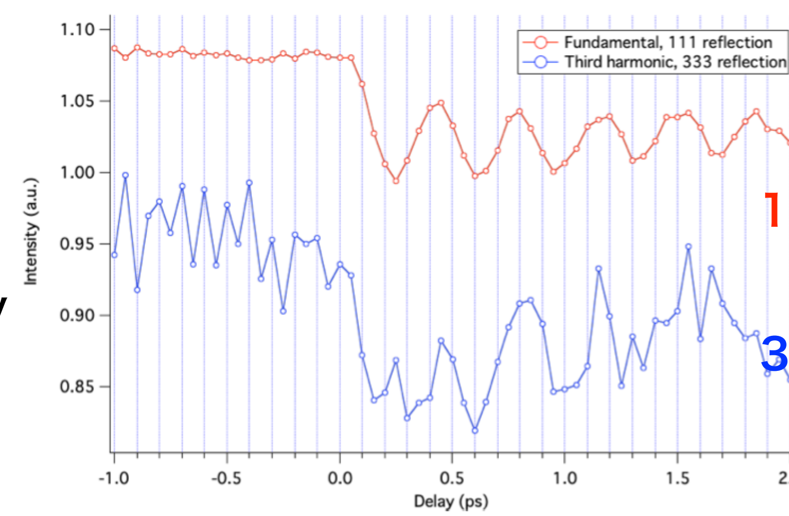
Seeding condition keeps ± 5 eV

cf. Bandwidth of XFEL beam impinges on the seed crystal: ~10 eV

☑Experiments with harmonics of seeded-XFEL



b.w. of 13 eV @27 keV



XPP of bismuth

coherent phonons induced by optical laser

111 reflection measured w/ fundamental (9 keV)

333 reflection measured w/ third harmonic (27 keV)

☑Tailoring electron-beam for self-seeding (not started yet)

- Parameter tuning of accelerator based on spectral brightness and/or new RF deflector combined with machine learning

Summary

- A new seeding scheme using a micro channel-cut crystal, called *"reflection self-seeding"*, was implemented at SACLA and works pretty well.

- The gain of spectral brightness compared with SASE-XFEL is typically 7-8, but sometimes reaches ~10 (Si 220).

- Tuning time of self-seeding is ~8 hours and seeding condition keeps over 3 days.

- Seeded-XFELs are now provided for user experiments as a standard operation mode of SACLA.

- Fast photon energy scan, evaluate and use of harmonics of seeded-XFEL, and further improve of spectral brightness by tailoring electron beam qualities are our on-going projects.

Thanks to…

SACLA SPring-8

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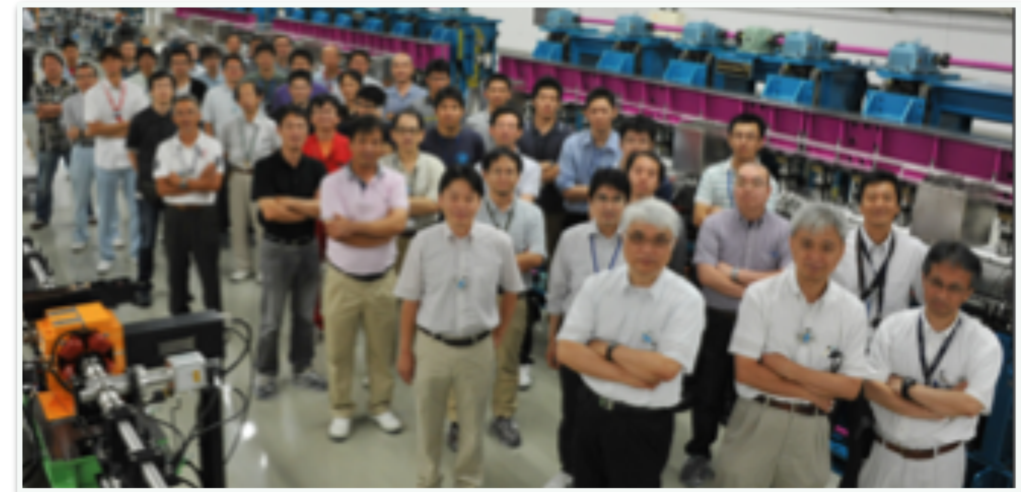

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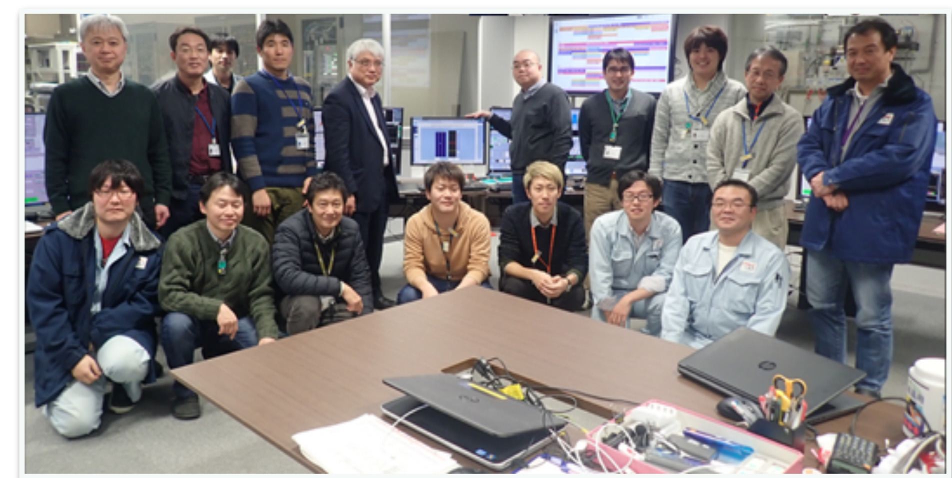

SLAC NATIONAL ACCELERATOR LABORATORY

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TOYAMA

株式会社 サートンワークス

Thank you
for your attention!