Hard x-ray self-seeding at the LCLS

Ryan R. Lindberg, on behalf of the Hard X-Ray Self-Seeding team
Advanced Photon Source, Argonne National Laboratory

34th International Free-Electron Laser Conference
August 27, 2012

FEL 2012 NARA

34th International
Free Electron Laser Conference
26-31 August 2012
Nara Prefectural New Public Hall, Nara, Japan

The Advanced Photon Source is an Office of Science User Facility operated for the U.S. Department of Energy Office of Science by Argonne National Laboratory

Acknowledgments

- The HXRSS team – a collaboration of SLAC National Lab, the Advanced Photon Source (APS) at Argonne National Lab, and the Technological Institute for Superhard and Novel Carbon Materials (TISNCM, Troitsk, Russia)

  J. Amann, F.-J. Decker, Y. Ding, P. Emma (LBNL) Y. Feng, J. Frisch, D. Fritz, J. Hastings, Z. Huang, J. Krzywinski, H. Loos, A. Lutman, H.-D. Nuhn, D. Ratner, J. Rzepiela, S. Spampinati (ELETTRA, Basovizza), D. Walz, J. Welch, J. Wu, and D. Zhu

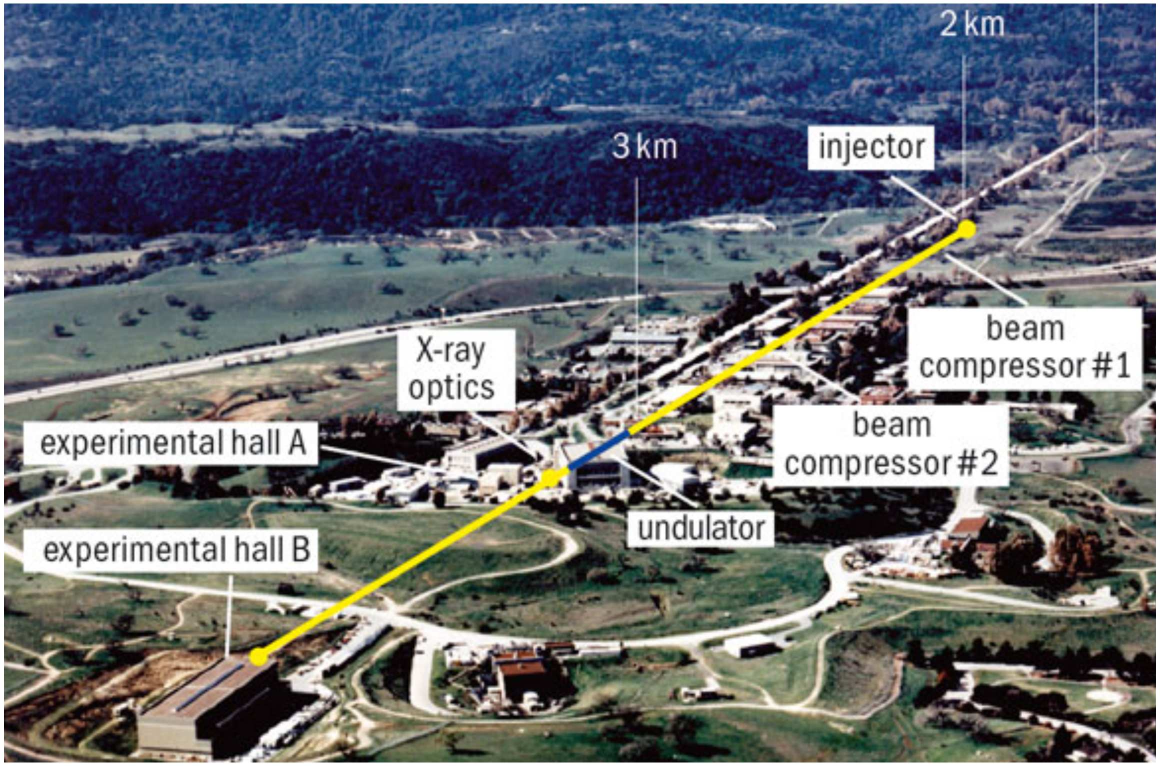
  W. Berg, D. Shu, Yu. Shvyd'ko, S. Stoupin, E. Trakhtenberg, and A. Zholents

  V. Blank and S.Terentiev

- Engineers and technicians @ SLAC & APS, and the LCLS operators
- Colleagues at DESY – G. Geloni, V. Kocharyan, and E. Saldin

The LCLS has produced intense Self-Amplified Spontaneous Emission (SASE) x-rays since 2009

- X-rays with wavelengths from 1.2 – 25 Å
- Up to 3 mJ/pulse ($\sim 10^{12}$ photons/pulse)
- 120 Hz rep rate
- Variable pulse length from few – 100 fs
- $\Delta\omega/\omega \sim 10^{-3}$



Flagship applications include:
Single shot x-ray imaging, Nonlinear physics, and Femtosecond dynamics

The LCLS enables new scientific inquiries/discoveries

LETTER

doi:10.1038/nature09750

Femtosecond X-ray protein nanocrystallography

Henry N. Chapman[1,2], Petra Fromme[3], Anton Barty[1], Thomas A. White[1], Richard A. Kirian[4], Andrew Aquila[1], Mark S. Hunter[3], Joachim Schulz[1], Daniel P. DePonte[1], Uwe Weierstall[4], R. Bruce Doak[4], Filipe R. N. C. Maia[5], Andrew V. Martin[1], Ilme Schlichting[6,7], Lukas Lomb[7], Nicola Coppola[1]†, Robert L. Shoeman[7], Sascha W. Epp[6,8], Robert Hartmann[9], Daniel Rolles[6,7], Artem Rudenko[6,8], Lutz Foucar[6,7], Nils Kimmel[10], Georg Weidenspointner[11,10], Peter Holl[9], Mengning Liang[1], Miriam Barthelmess[12], Carl Caleman[1], Sébastien Boutet[13], Michael J. Bogan[14], Jacek Krzywinski[13], Christoph Bostedt[13], Saša Bajt[12], Lars Gumprecht[1], Benedikt Rudek[6,8], Benjamin Erk[6,8], Carlo Schmidt[6,8], André Hömke[6,8], Christian Reich[9], Daniel Pietschner[10], Lothar Strüder[6,10], Günter Hauser[10], Hubert Gorke[15], Joachim Ullrich[6,8], Sven Herrmann[10], Gerhard Schaller[10], Florian Schopper[10], Heike Soltau[9], Kai-Uwe Kühnel[8], Marc Messerschmidt[13], John D. Bozek[13], Stefan P. Hau-Riege[16], Matthias Frank[16], Christina Y. Hampton[14], Raymond G. Sierra[14], Dmitri Starodub[14], Garth J. Williams[13], Janos Hajdu[5], Nicusor Timneanu[5], M. Marvin Seibert[5]†, Jakob Andreasson[5], Andrea Rocker[5], Olof Jönsson[5], Martin Svenda[5], Stephan Stern[1], Karol Nass[2], Robert Andritschke[10], Claus-Dieter Schröter[8], Faton Krasniqi[6,7], Mario Bott[7], Kevin E. Schmidt[4], Xiaoyu Wang[4], Ingo Grotjohann[3], James M. Holton[17], Thomas R. M. Barends[7], Richard Neutze[18], Stefano Marchesini[17], Raimund Fromme[3], Sebastian Schorb[19], Daniela Rupp[19], Marcus Adolph[19], Tais Gorkhover[19], Inger Andersson[20], Helmut Hirsemann[12], Guillaume Potdevin[12], Heinz Graafsma[12], Björn Nilsson[12] & John C. H. Spence[4]

X-ray crystallography provides the vast majority of macromolecular structures, but the success of the method relies on growing crystals of sufficient size. In conventional measurements, the necessary increase in X-ray dose to record data from crystals that are too small leads to extensive damage before a diffraction signal can be recorded[1–3]. It is particularly challenging to obtain large, well-diffracting crystals of membrane proteins, for which fewer than 300 unique structures have been determined despite their importance in all living cells. Here we present a method for structure determination where single-crystal X-ray diffraction 'snapshots' are collected from a fully hydrated stream of nanocrystals using femtosecond pulses from a hard-X-ray free-electron laser, the Linac Coherent Light Source[4]. We prove this concept with nanocrystals of photosystem I, one of the largest membrane protein complexes[5]. More than 3,000,000 diffraction patterns were collected in this study, and a three-dimensional data set was assembled from individual photosystem I nanocrystals (~200 nm to 2 μm in size). We mitigate the problem of radiation damage in crystallography by using pulses briefer than the timescale of most damage processes[6]. This offers a new approach to structure determination of macromolecules that do not yield crystals of sufficient size for studies using conventional radiation sources or are particularly sensitive to radiation damage.

PRL **104,** 253002 (2010) PHYSICAL REVIEW LETTERS week ending 25 JUNE 2010

Ultraintense X-Ray Induced Ionization, Dissociation, and Frustrated Absorption in Molecular Nitrogen

M. Hoener,[1,2] L. Fang,[1] O. Kornilov,[3] O. Gessner,[3] S. T. Pratt,[4] M. Gühr,[5] E. P. Kanter,[4] C. Blaga,[6] C. Bostedt,[7] J. D. Bozek,[7] P. H. Bucksbaum,[5] C. Buth,[5,8] M. Chen,[9] R. Coffee,[7] J. Cryan,[5] L. DiMauro,[6] M. Glownia,[5] E. Hosler,[10] E. Kukk,[11] S. R. Leone,[3,10] B. McFarland,[5] M. Messerschmidt,[7] B. Murphy,[1] V. Petrovic,[5] D. Rolles,[12] and N. Berrah[1,*]

[1]Western Michigan University Physics Department, Kalamazoo, Michigan 49008, USA
[2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
[3]Ultrafast X-ray Science Laboratory Chemical Sciences Division Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
[4]Argonne National Laboratory, Argonne, Illinois 60439, USA
[5]The PULSE Institute for Ultrafast Energy Science, SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA
[6]The Ohio State University, Department of Physics, Columbus, Ohio 43210, USA
[7]Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA
[8]Department of Physics, Louisiana State University, Baton Rouge, Louisiana 70803, USA
[9]Lawrence Livermore National Laboratory, Livermore, California 94550, USA
[10]Departments of Chemistry and Physics University of California, Berkeley, California 94710, USA
[11]Department of Physics and Astronomy, University of Turku 20014 Turku, Finland
[12]Max Planck Advanced Study Group, CFEL, 22761 Hamburg, Germany

(Received 24 May 2010; published 23 June 2010)

is studied with femtosecond time
picture of intense x-ray induced

Science AAAS

High-Resolution Protein Structure Determination by Serial Femtosecond Crystallography
Sébastien Boutet *et al.*
Science **337**, 362 (2012);
DOI: 10.1126/science.1217737

High-Resolution Protein Structure Determination by Serial Femtosecond Crystallography

Sébastien Boutet,[1*] Lukas Lomb,[2,3] Garth J. Williams,[1] Thomas R. M. Barends,[2,3] Andrew Aquila,[4] R. Bruce Doak,[5] Uwe Weierstall,[5] Daniel P. DePonte,[4] Jan Steinbrener,[2,3] Robert L. Shoeman,[2,3] Marc Messerschmidt,[1] Anton Barty,[4] Thomas A. White,[4] Stephan Kassemeyer,[2,3] Richard A. Kirian,[5] M. Marvin Seibert,[1] Paul A. Montanez,[1] Chris Kenney,[6] Ryan Herbst,[6] Philip Hart,[6] Jack Pines,[6] Gunther Haller,[6] Sol M. Gruner,[7,8] Hugh T. Philipp,[7] Mark W. Tate,[7] Marianne Hromalik,[9] Lucas J. Koerner,[10] Niels van Bakel,[11] John Morse,[12] Wilfred Ghonsalves,[1] David Arnlund,[13] Michael J. Bogan,[14] Carl Caleman,[4] Raimund Fromme,[15] Christina Y. Hampton,[14] Mark S. Hunter,[15] Linda C. Johansson,[13] Gergely Katona,[13] Christopher Kupitz,[15] Mengning Liang,[4] Andrew V. Martin,[4] Karol Nass,[16] Lars Redecke,[17,18] Francesco Stellato,[4] Nicusor Timneanu,[19] Dingjie Wang,[5] Nadia A. Zatsepin,[5] Donald Schafer,[1] James Defever,[1] Richard Neutze,[13] Petra Fromme,[15] John C. H. Spence,[5] Henry N. Chapman,[4,16] Ilme Schlichting[2,3]

Structure determination of proteins and other macromolecules has historically required the growth of high-quality crystals sufficiently large to diffract x-rays efficiently while withstanding radiation damage. We applied serial femtosecond crystallography (SFX) using an x-ray free-electron laser (XFEL) to obtain high-resolution structural information from microcrystals (less than 1 micrometer by 1 micrometer by 3 micrometers) of the well-characterized model protein lysozyme. The agreement with synchrotron data demonstrates the immediate relevance of SFX for analyzing the structure of the large group of difficult-to-crystallize molecules.

LETTER

doi:10.1038/nature09748

Single mimivirus particles intercepted and imaged with an X-ray laser

M. Marvin Seibert[1]*, Tomas Ekeberg[1]*, Filipe R. N. C. Maia[1]*, Martin Svenda[1], Jakob Andreasson[1], Olof Jönsson[1], Duško Odić[1], Bianca Iwan[1], Andrea Rocker[1], Daniel Westphal[1], Max Hantke[1], Daniel P. DePonte[2], Anton Barty[2], Joachim Schulz[2], Lars Gumprecht[2], Nicola Coppola[2], Andrew Aquila[2], Mengning Liang[2], Thomas A. White[2], Andrew Martin[2], Carl Caleman[1,2], Stephan Stern[2,3], Chantal Abergel[4], Virginie Seltzer[4], Jean-Michel Claverie[4], Christoph Bostedt[5], John D. Bozek[5], Sébastien Boutet[5], A. Alan Miahnahri[5], Marc Messerschmidt[5], Jacek Krzywinski[5], Garth Williams[5], Keith O. Hodgson[6], Michael J. Bogan[6], Christina Y. Hampton[6], Raymond G. Sierra[6], Dmitri Starodub[6], Inger Andersson[7], Saša Bajt[8], Miriam Barthelmess[8], John C. H. Spence[9], Petra Fromme[10], Uwe Weierstall[9], Richard Kirian[9], Mark Hunter[10], R. Bruce Doak[9], Stefano Marchesini[11], Stefan P. Hau-Riege[12], Matthias Frank[12], Robert L. Shoeman[13], Lukas Lomb[13], Sascha W. Epp[14,15], Robert Hartmann[16], Daniel Rolles[13,14], Artem Rudenko[14,15], Carlo Schmidt[14,15], Lutz Foucar[13,14], Nils Kimmel[17,18], Peter Holl[16], Benedikt Rudek[14,15], Benjamin Erk[14,15], André Hömke[14,15], Christian Reich[16], Daniel Pietschner[17,18], Georg Weidenspointner[17,18], Lothar Strüder[14,17,18,19], Günter Hauser[17,18], Hubert Gorke[20], Joachim Ullrich[14,15], Ilme Schlichting[13,14], Sven Herrmann[17,18], Gerhard Schaller[17,18], Florian Schopper[17,18], Heike Soltau[16], Kai-Uwe Kühnel[15], Robert Andritschke[17,18], Claus-Dieter Schröter[15], Faton Krasniqi[13,14], Mario Bott[13], Sebastian Schorb[21], Daniela Rupp[21], Marcus Adolph[21], Tais Gorkhover[21], Helmut Hirsemann[8], Guillaume Potdevin[8], Heinz Graafsma[8], Björn Nilsson[8], Henry N. Chapman[2,3] & Janos Hajdu[1]

X-ray lasers offer new capabilities in understanding the structure of biological systems, complex materials and matter under extreme conditions[1–4]. Very short and extremely bright, coherent X-ray pulses can be used to outrun key damage processes and obtain a single diffraction pattern from a large macromolecule, a virus or a cell before the sample explodes and turns into plasma[1]. The continuous diffraction pattern of non-crystalline objects permits oversampling and direct phase retrieval[2]. Here we show that high-quality diffraction data can be obtained with a single X-ray pulse from a non-crystalline biological sample, a single mimivirus particle, which was injected into the pulsed beam of a hard-X-ray free-electron laser, the Linac Coherent Light Source[5]. Calculations indicate that the energy deposited into the virus by the pulse heated the particle to over 100,000 K after the pulse had left the sample. The reconstructed exit wavefront (image) yielded 32-nm full-period resolution in a single exposure and showed no measurable damage. The reconstruction indicates inhomogeneous arrangement of dense material inside the virion. We expect that significantly higher resolutions will be achieved in such experiments with shorter and brighter photon pulses focused to a smaller area. The resolution in such experiments can be further extended for samples available in multiple identical copies.

an X-r
require
Mim
known
(in fact,
viral ca
and is c
the part
full thre
its fibril
(compa
though
of the p
smaller
of a vir
are caus
about t
Figu
virus pa
was m
ment[12]
line[13] at

Time-resolved pump-probe experiments at the LCLS

James M. Glownia,[1,2,*] J. Cryan,[1,3] J. Andreasson,[4] A. Belkacem,[5] N. Berrah,[6] C. I. Blaga,[7] C. Bostedt,[8] J. Bozek,[8] L. F. DiMauro,[7] L. Fang,[6] J. Frisch,[8] O. Gessner,[5] M. Gühr,[1] J. Hajdu,[4] M. P. Hertlein,[10] M. Hoener,[6,10] G. Huang,[10] O. Kornilov,[5] J. P. Marangos,[11] A. M. March,[12] B. K. McFarland,[1,2] H. Merdji,[1,13] V. S. Petrovic,[3] C. Raman,[14] D. Ray,[12,15] D. A. Reis,[1,2] M. Trigo,[1] J. L. White,[2] W. White,[8] R. Wilcox,[10] L. Young,[12]
R. N. Coffee,[1,8] and P. H. Bucksbaum,[1,2,3]

#128707 - $15.00 USD Received 21 May 2010; revised 3 Jul 2010; accepted 24 Jul 2010; published 2 Aug 2010

16 August 2010 / Vol. 18, No. 17 / OPTICS EXPRESS 17620

nature
Vol 466 | 1 July 2010 | **doi:10.1038/nature09177**

ARTICLES

Femtosecond electronic response of atoms to ultra-intense X-rays

L. Young[1], E. P. Kanter[1], B. Krässig[1], Y. Li[1], A. M. March[1], S. T. Pratt[1], R. Santra[1,2], S. H. Southworth[1], N. Rohringer[3], L. F. DiMauro[4], G. Doumy[4], C. A. Roedig[4], N. Berrah[5], L. Fang[5], M. Hoener[5,6], P. H. Bucksbaum[7], J. P. Cryan[7], S. Ghimire[7], J. M. Glownia[7], D. A. Reis[7], J. D. Bozek[8], C. Bostedt[8] & M. Messerschmidt[8]

An era of exploring the interactions of high-intensity, hard X-rays with matter has begun with the start-up of a hard-X-ray free-electron laser, the Linac Coherent Light Source (LCLS). Understanding how electrons in matter respond to ultra-intense X-ray radiation is essential for all applications. Here we reveal the nature of the electronic response of a free atom to unprecedented high-intensity, short-wavelength, high-fluence radiation (respectively 10^{18} W cm^{-2}, 1.5–0.6 nm, ~10^5 X-ray photons per Å^2). At this fluence, the neon target inevitably changes during the course of a single femtosecond-duration X-ray pulse—by sequentially ejecting electrons—to produce fully-stripped neon through absorption of six photons. Rapid photoejection of inner-shell electrons produces 'hollow' atoms and an intensity-induced X-ray transparency. Such transparency, due to the presence of inner-shell vacancies, can be induced in all atomic, molecular and condensed matter systems at high intensity. Quantitative comparison with theory allows us to extract LCLS fluence and pulse duration. Our successful modelling of X-ray/atom interactions using a straightforward rate equation approach augurs favourably for extension to complex systems.

Selected for a Viewpoint in *Physics*

PRL **109,** 065002 (2012) PHYSICAL REVIEW LETTERS week ending 10 AUGUST 2012

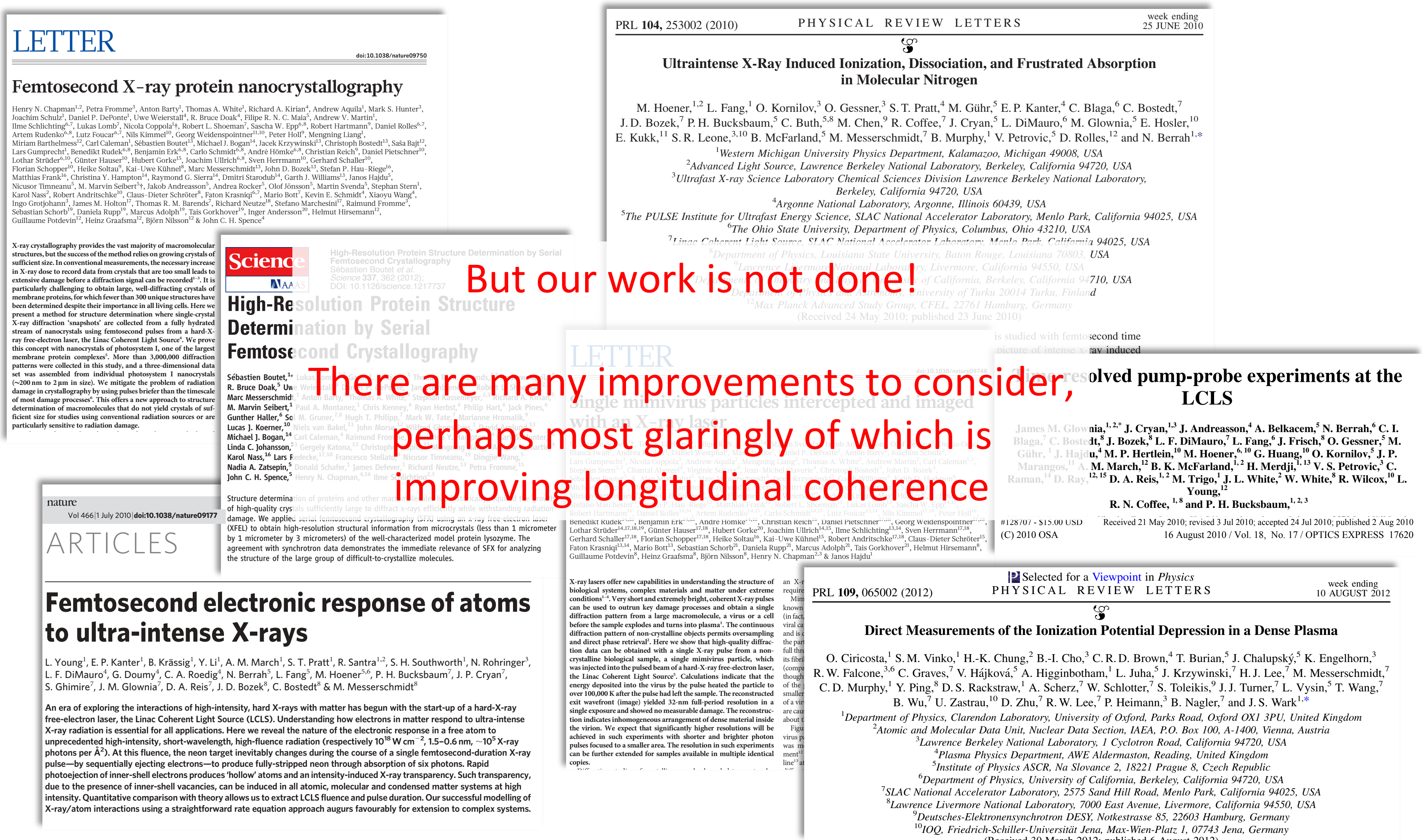
Direct Measurements of the Ionization Potential Depression in a Dense Plasma

O. Ciricosta,[1] S. M. Vinko,[1] H.-K. Chung,[2] B.-I. Cho,[3] C. R. D. Brown,[4] T. Burian,[5] J. Chalupský,[5] K. Engelhorn,[3] R. W. Falcone,[3,6] C. Graves,[7] V. Hájková,[5] A. Higginbotham,[1] L. Juha,[5] J. Krzywinski,[7] H. J. Lee,[7] M. Messerschmidt,[7] C. D. Murphy,[1] Y. Ping,[8] D. S. Rackstraw,[1] A. Scherz,[7] W. Schlotter,[7] S. Toleikis,[9] J. J. Turner,[7] L. Vysin,[5] T. Wang,[7] B. Wu,[7] U. Zastrau,[10] D. Zhu,[7] R. W. Lee,[7] P. Heimann,[3] B. Nagler,[7] and J. S. Wark[1,*]

[1]Department of Physics, Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom
[2]Atomic and Molecular Data Unit, Nuclear Data Section, IAEA, P.O. Box 100, A-1400, Vienna, Austria
[3]Lawrence Berkeley National Laboratory, 1 Cyclotron Road, California 94720, USA
[4]Plasma Physics Department, AWE Aldermaston, Reading, United Kingdom
[5]Institute of Physics ASCR, Na Slovance 2, 18221 Prague 8, Czech Republic
[6]Department of Physics, University of California, Berkeley, California 94720, USA
[7]SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA
[8]Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore, California 94550, USA
[9]Deutsches-Elektronensynchrotron DESY, Notkestrasse 85, 22603 Hamburg, Germany
[10]IOQ, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

(Received 30 March 2012; published 6 August 2012)

The LCLS enables new scientific inquiries/discoveries



But our work is not done!

There are many improvements to consider, perhaps most glaringly of which is improving longitudinal coherence

The need to seed

- SASE is initiated by electron beam shot noise

  → many longitudinal modes & normalized bandwidth $\Delta\omega/\omega \sim \rho$
- Longitudinal coherence/spectral brightness can be improved by seeding the FEL with a coherent signal at the wavelength of interest
- Motivation from experimental users may include

  1. Increase spectral brightness

     Increase number of photons in a specified narrow bandwidth

     Decrease noise signals due to nearby spectral components

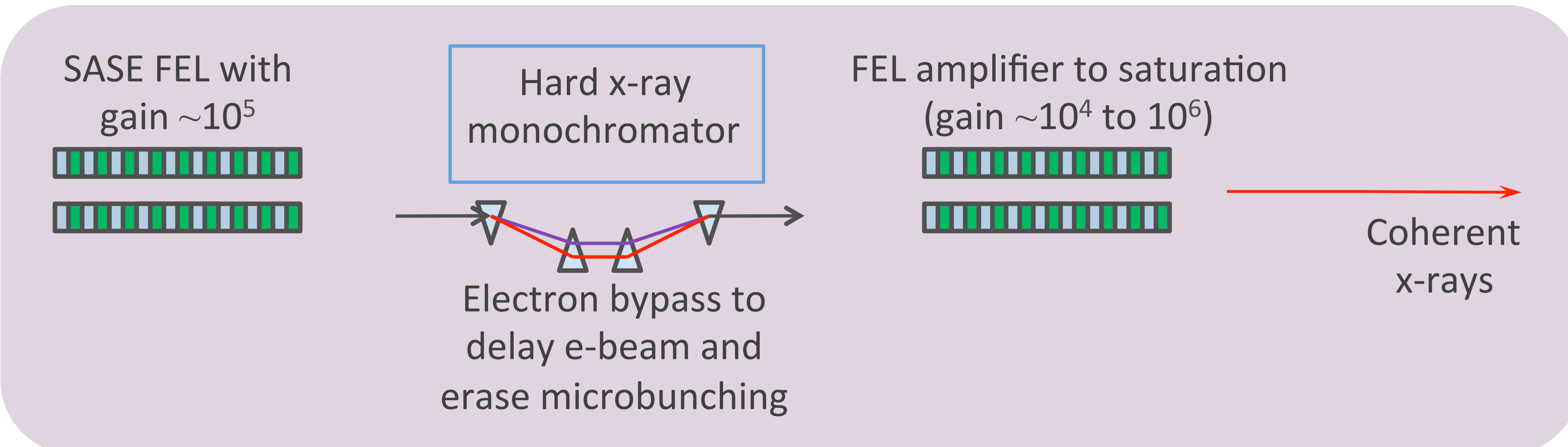
  2. Produce temporally coherent x-rays

  3. Increase total number of photons by judicious tapering

     Seeded field saturates more uniformly, and tapering the undulator strength can more efficiently extract additional energy from the e-beam

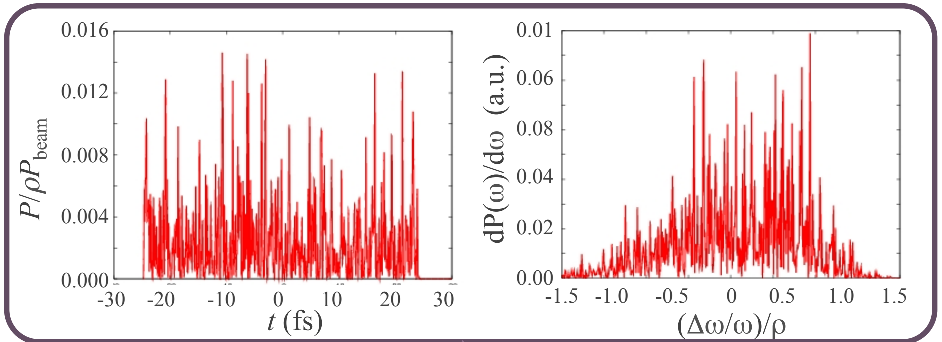
Self-seeding

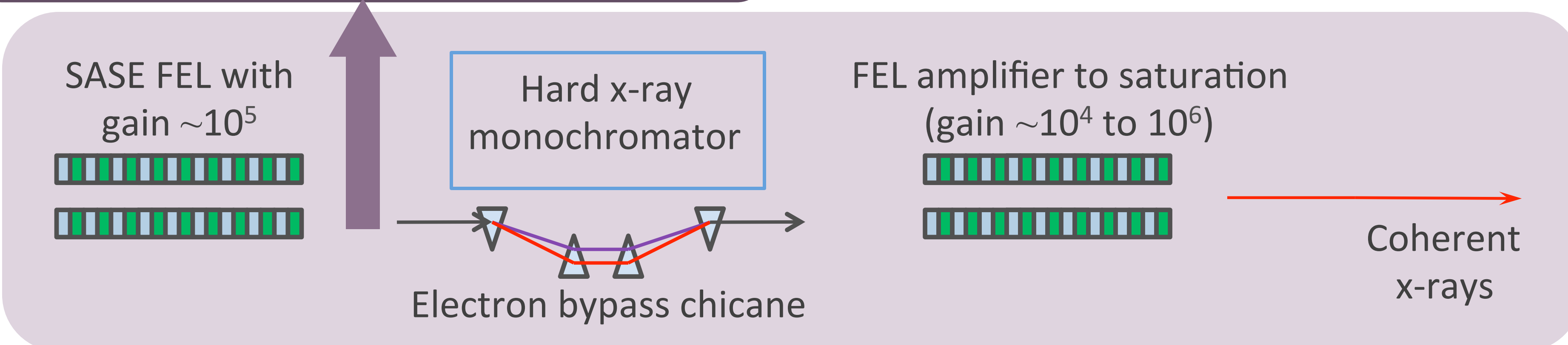
Self-seeding uses SASE + monochromator to generate coherent seed



E.L. Saldin, E.A. Schneidmiller, Yu.V. Shvyd'ko, and M.V. Yurkov, *NIMA* **475**, 357 (2001)
Y. Ding, Z. Huang, and R. D. Ruth, *Phys. Rev. ST Accel. Beams* **13**, 060703 (2010)
G. Geloni, V. Kocharyan, and E.L. Saldin, *J. Modern Optics* **58**, 1391 (2011)

Self-seeding

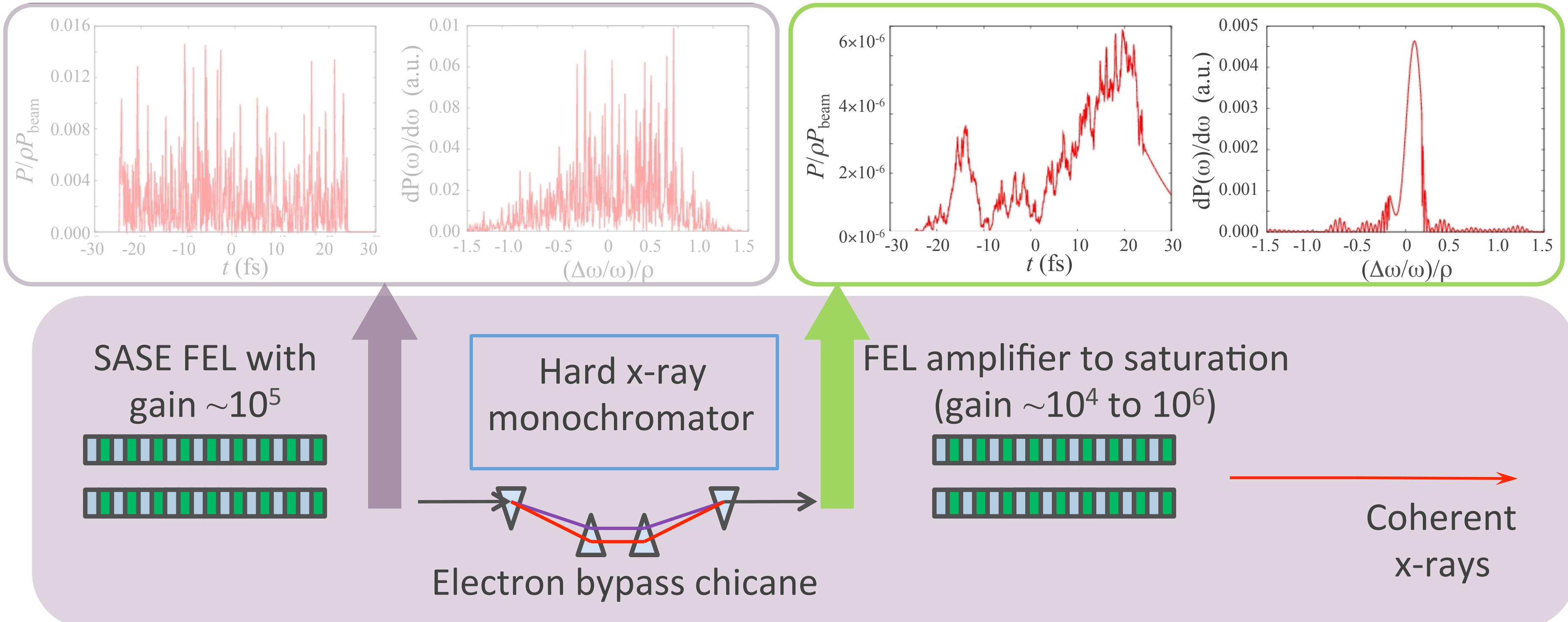




- Power large enough so that monochromatic signal dominates the seeding of SASE by electron beam shot noise
- FEL-induced energy spread on beam must remain small (well before nonlinear regime)

Example uses LCLS-type parameters with $\rho = 5\times10^{-4}$ and $(\Delta\omega/\omega)_{mono} = 2\times10^{-5}$

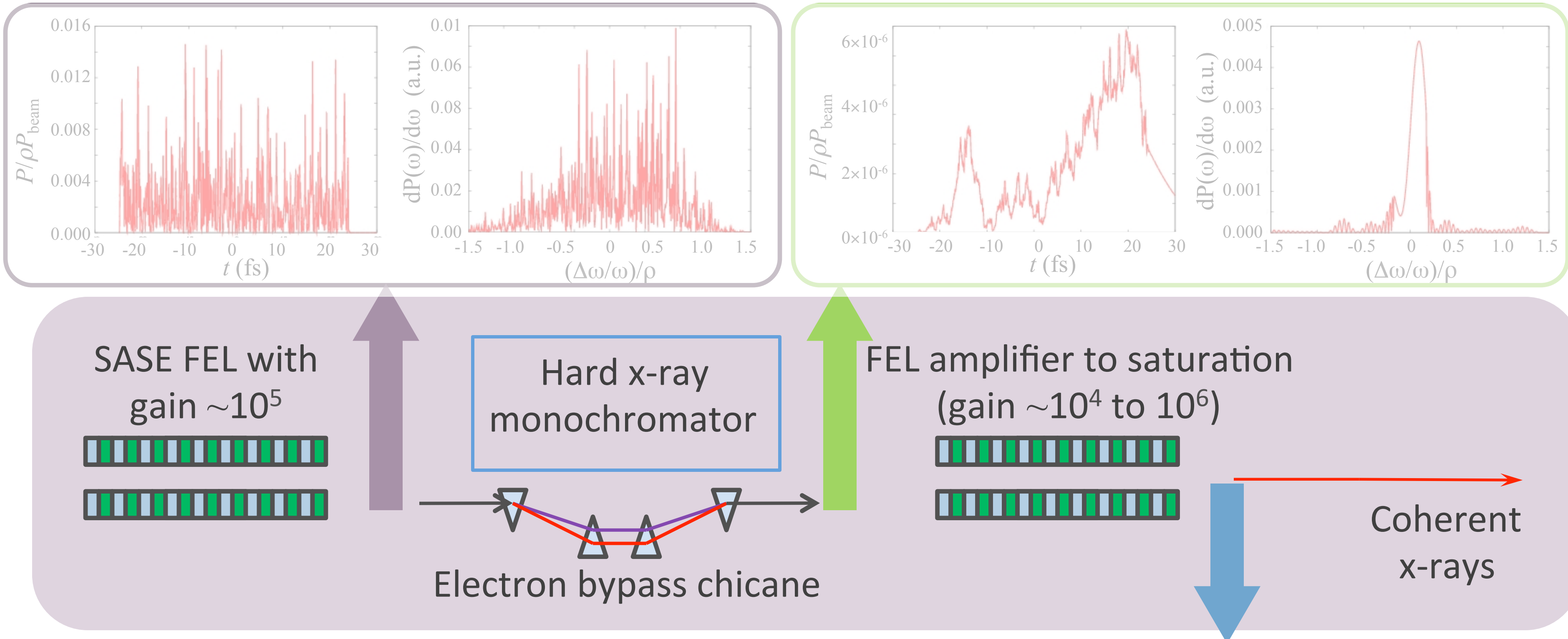
Self-seeding



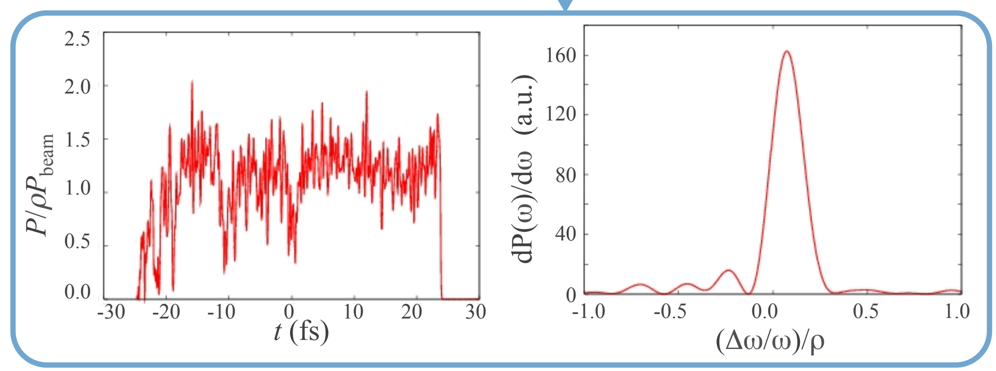
- Monochromator selects narrow bandwidth seed whose energy fluctuates by ~100%
- Electron beam is delayed to overlap and amplify radiation in downstream undulator
- Chicane erases microbunching of SASE

Example uses LCLS-type parameters with $\rho = 5\times10^{-4}$ and $(\Delta\omega/\omega)_{mono} = 2\times10^{-5}$

Self-seeding



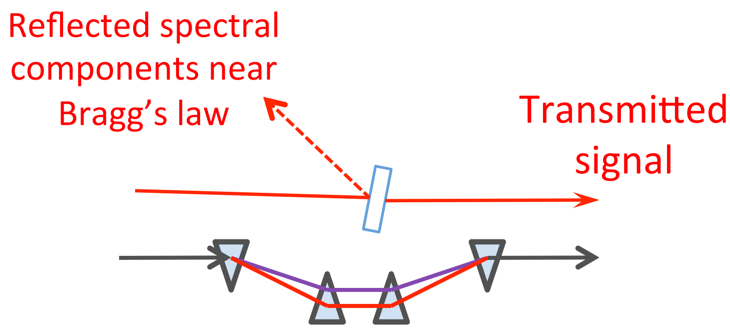
- Initial ~100% fluctuations of seed are reduced to ~20% at saturation
- Additional energy can be efficiently extracted by tapering the undulator strength after saturation



Wake monochromator for self-seeding of short x-ray pulses

Produces seed using time dependence of forward Bragg diffraction from a single crystal, i.e., time response of the crystal transmission function

Single crystal wake mono

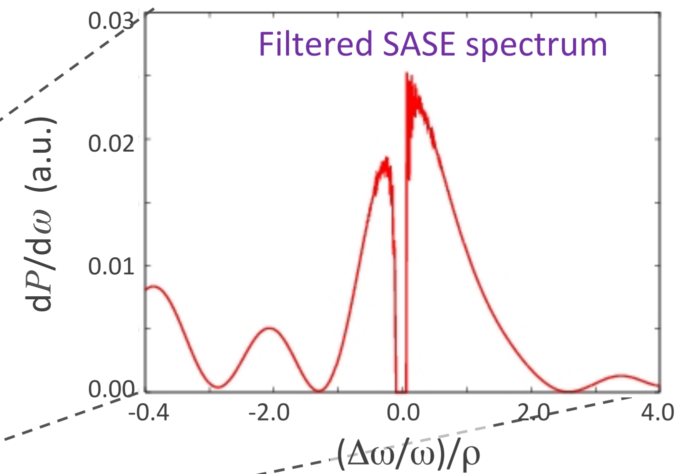


~3-4 m chicane washes out microbunching and delays electrons requires tens of fs

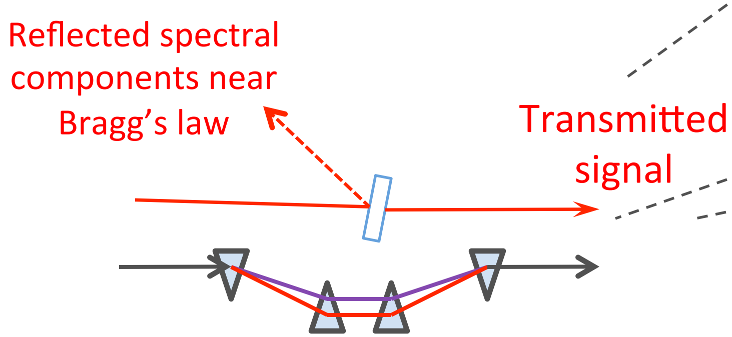
† G. Geloni, V. Kocharyan, and E.L. Saldin, *J. Modern Optics* **58**, 1391 (2011)

Wake monochromator for self-seeding of short x-ray pulses

Produces seed using time dependence of forward Bragg diffraction from a single crystal, i.e., time response of the crystal transmission function



Single crystal wake mono



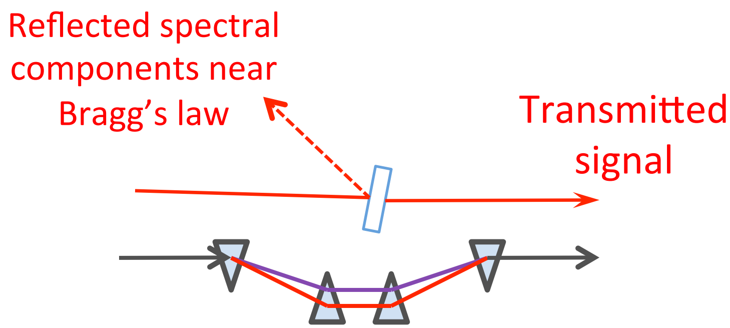
~3-4 m chicane washes out microbunching and delays electrons requires tens of fs

† G. Geloni, V. Kocharyan, and E.L. Saldin, *J. Modern Optics* **58**, 1391 (2011)

Wake monochromator for self-seeding of short x-ray pulses

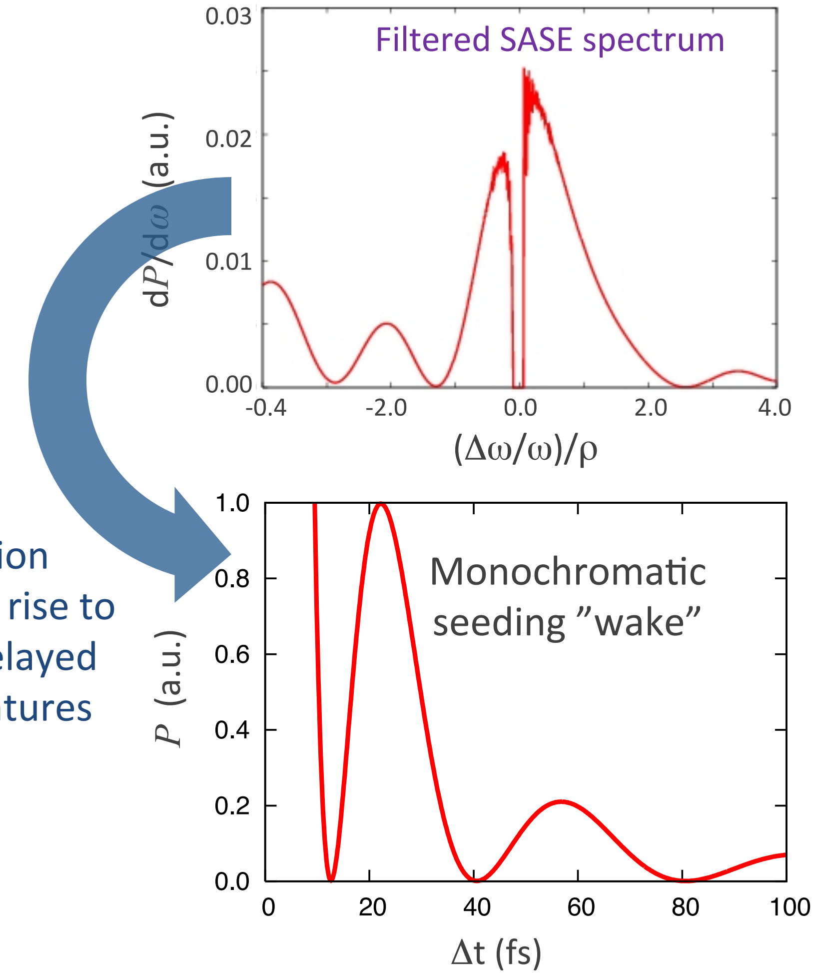
Produces seed using time dependence of forward Bragg diffraction from a single crystal, i.e., time response of the crystal transmission function

Single crystal wake mono



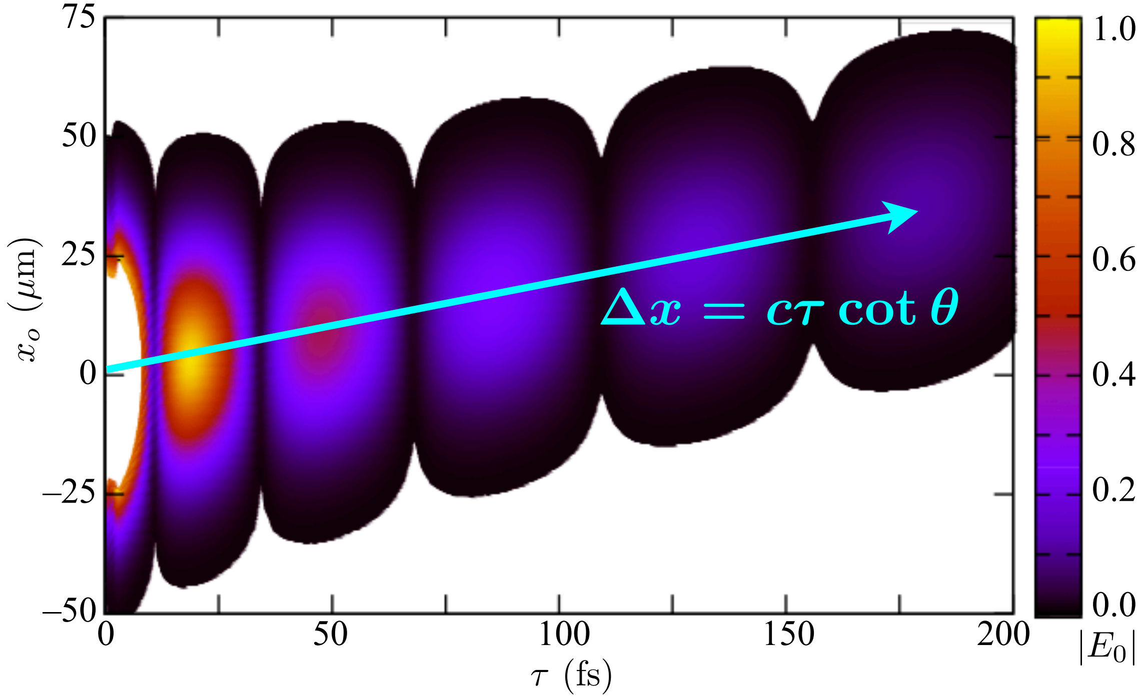
~3-4 m chicane washes out microbunching and delays electrons requires tens of fs

Transmission function gives rise to broad and delayed temporal features



† G. Geloni, V. Kocharyan, and E.L. Saldin, *J. Modern Optics* **58**, 1391 (2011)

Transverse displacement of self-seeding "wake"



Delayed seeding field is also transversely displaced according to $\Delta x = c\tau \cot\theta$

† R.R. Lindberg and Yu. Shvyd'ko, *Phys. Rev. ST-Accel. Beams* **15**, 050706 (2012)

Implementation at the LCLS

Great synthesis of wake monochromator idea with the fact that the LCLS can benefit from its conservative design – there's enough undulators for self-seeding to both produce and subsequently amplify its signal†

† G. Geloni, V. Kocharyan, and E.L. Saldin, "Cost-effective way to enhance the capabilities of the LCLS baseline," DESY 10-133, arXiv:1008.3036 (2010)

Implementation at the LCLS

Great synthesis of wake monochromator idea with the fact that the LCLS can benefit from its conservative design – there's enough undulators for self-seeding to both produce and subsequently amplify its signal†

Requirements for monochromator position:

1. Require enough SASE undulators to produce sufficient seeding power (1 MW >> 10 kW of effective SASE seeding from e-beam shot noise)
2. Limit SASE section so as to minimize energy spread increase/beam quality degradation due to the FEL process

† G. Geloni, V. Kocharyan, and E.L. Saldin, "Cost-effective way to enhance the capabilities of the LCLS baseline," DESY 10-133, arXiv:1008.3036 (2010)

Implementation at the LCLS

Great synthesis of wake monochromator idea with the fact that the LCLS can benefit from its conservative design – there's enough undulators for self-seeding to both produce and subsequently amplify its signal†

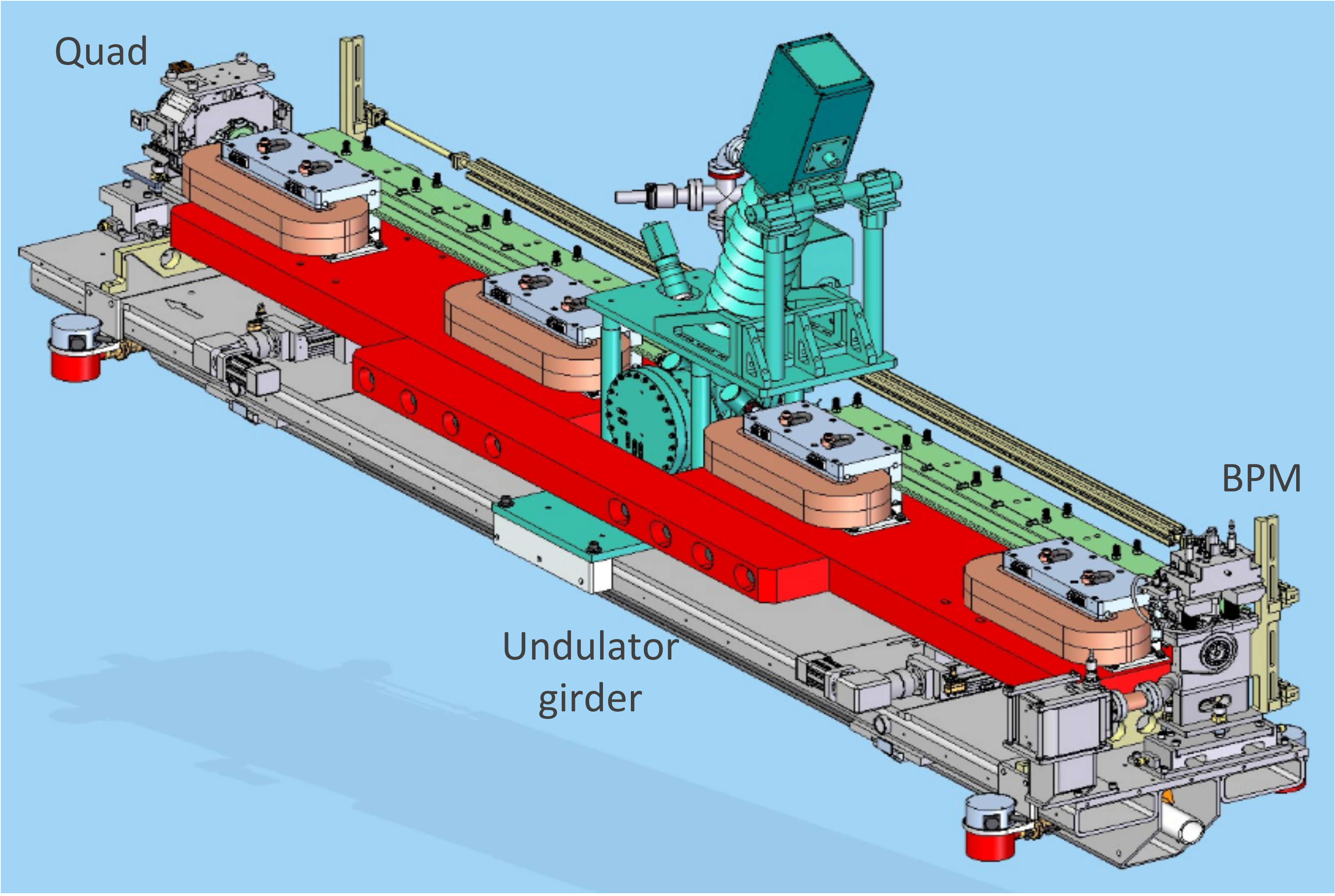
Requirements for monochromator position:

1. Require enough SASE undulators to produce sufficient seeding power (1 MW >> 10 kW of effective SASE seeding from e-beam shot noise)
2. Limit SASE section so as to minimize energy spread increase/beam quality degradation due to the FEL process

It was chosen to replace Undulator 16 with the monochromator system: 4-dipole chicane and the x-ray wake monochromator including diamond crystal in Bragg transmission

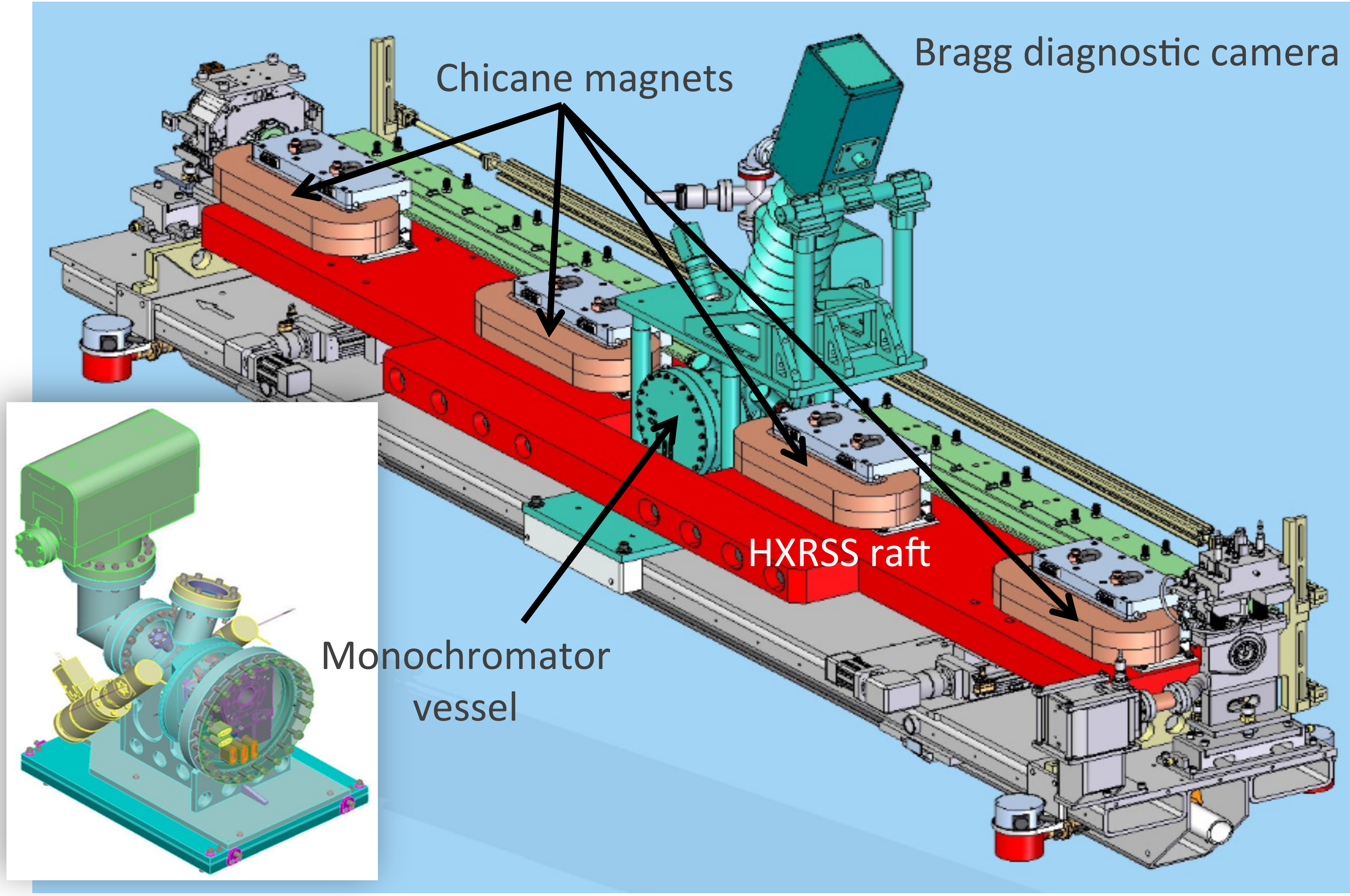
† G. Geloni, V. Kocharyan, and E.L. Saldin, "Cost-effective way to enhance the capabilities of the LCLS baseline," DESY 10-133, arXiv:1008.3036 (2010)

HXRSS design for Undulator 16



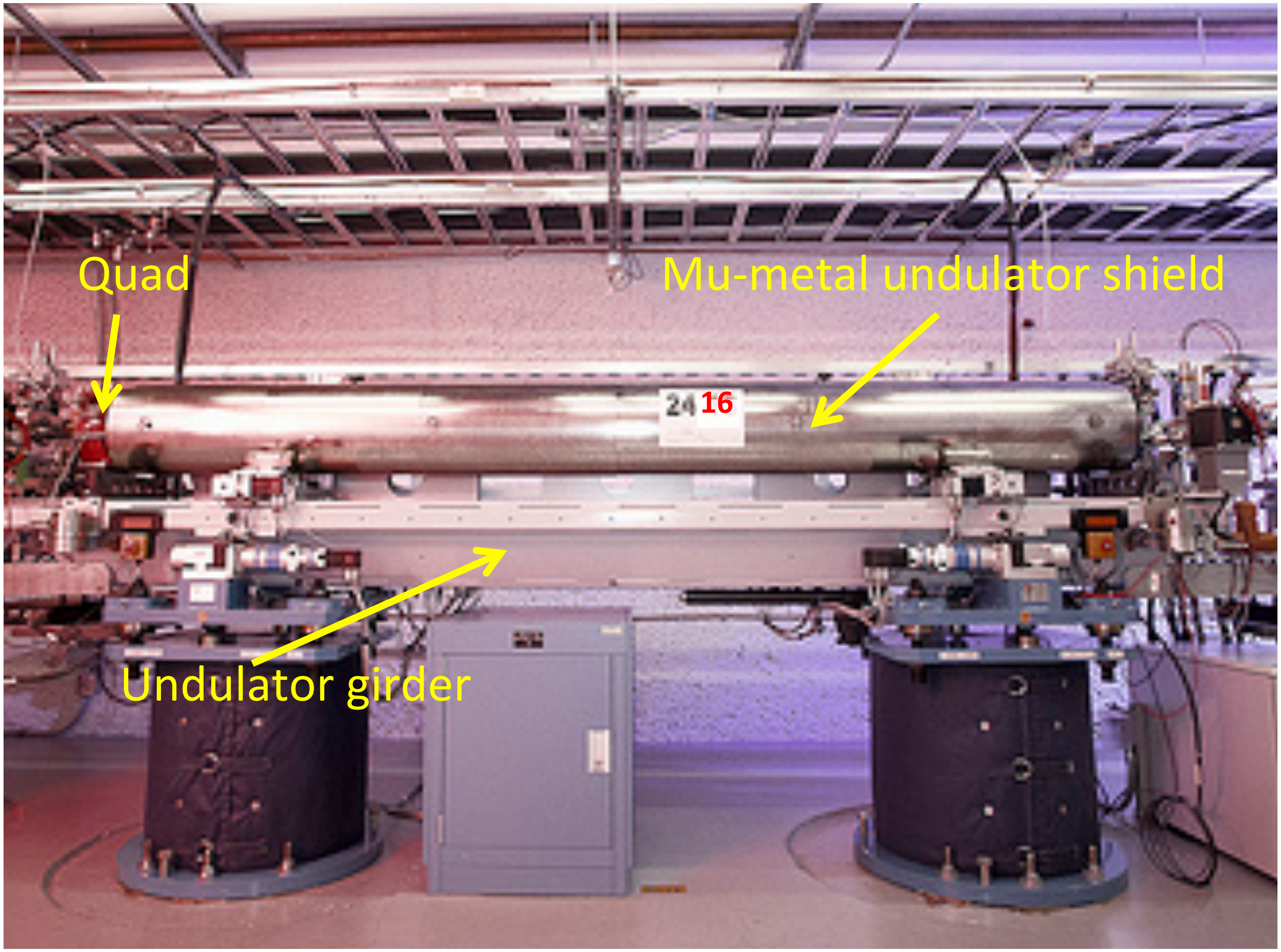
† Amman, Shultz, Trakhtenberg

HXRSS design for Undulator 16

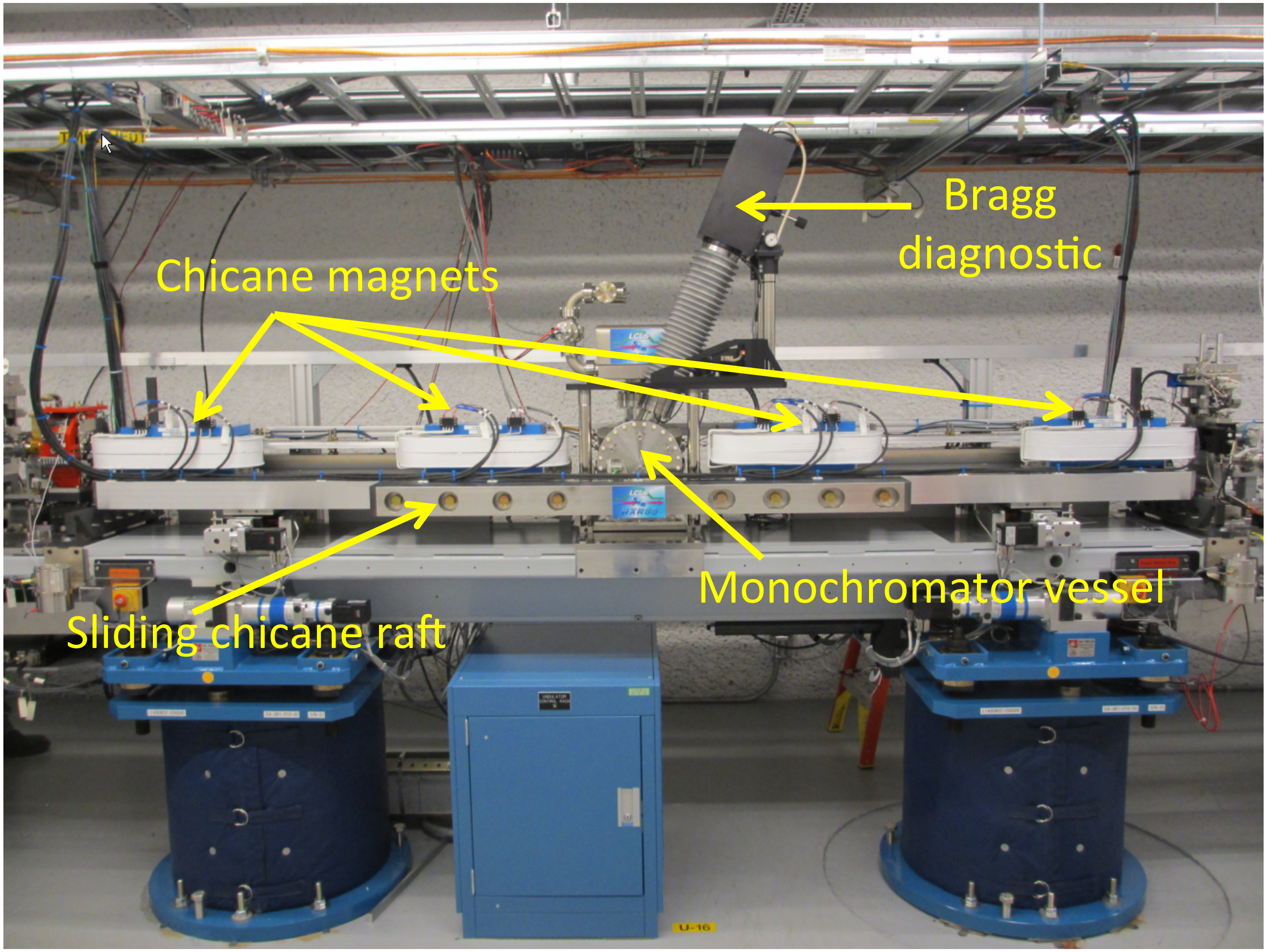


† Amman, Shultz, Trakhtenberg

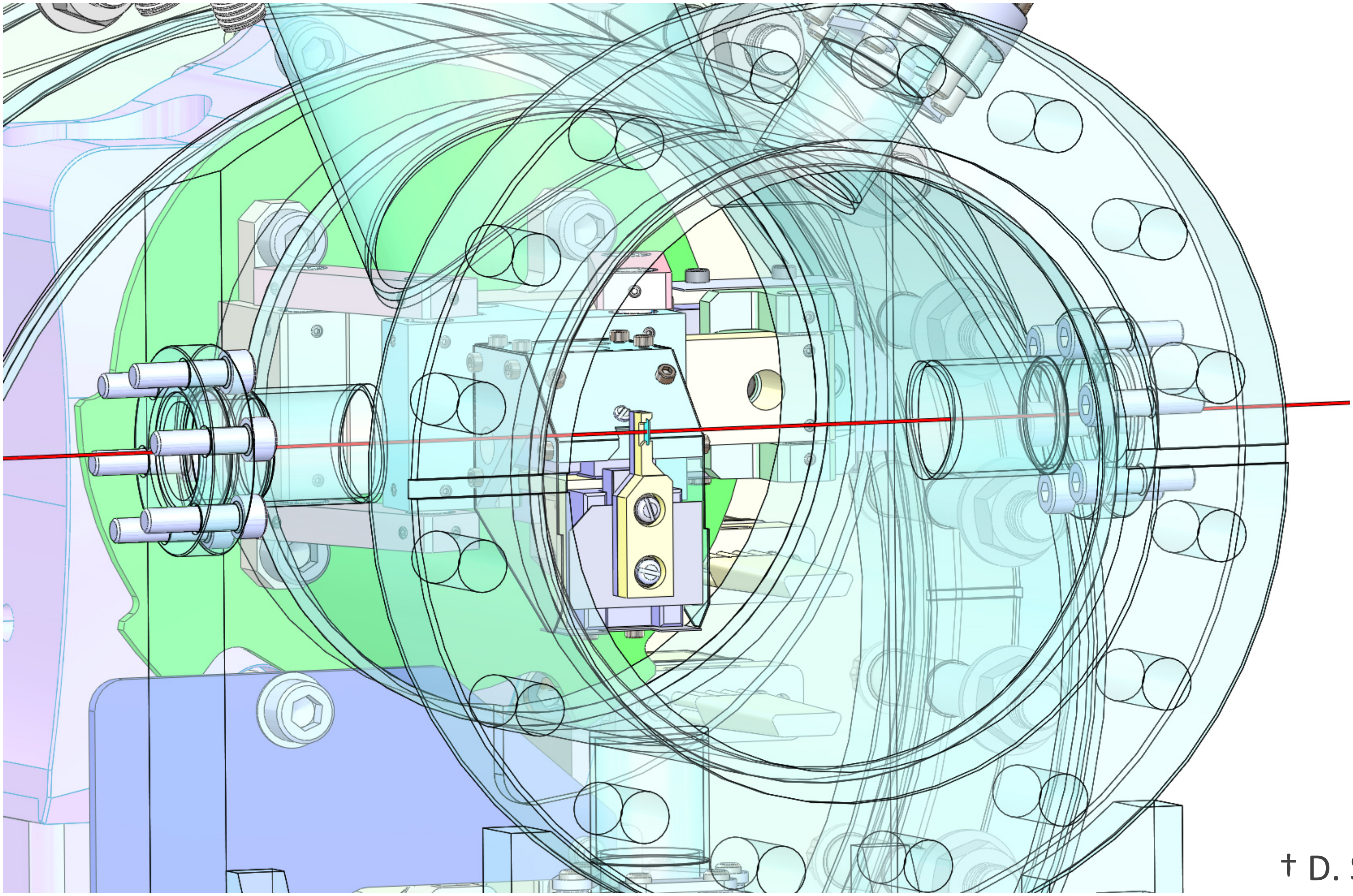
Standard LCLS undulator (of 33 total)



Monochromator and chicane @ Undulator 16

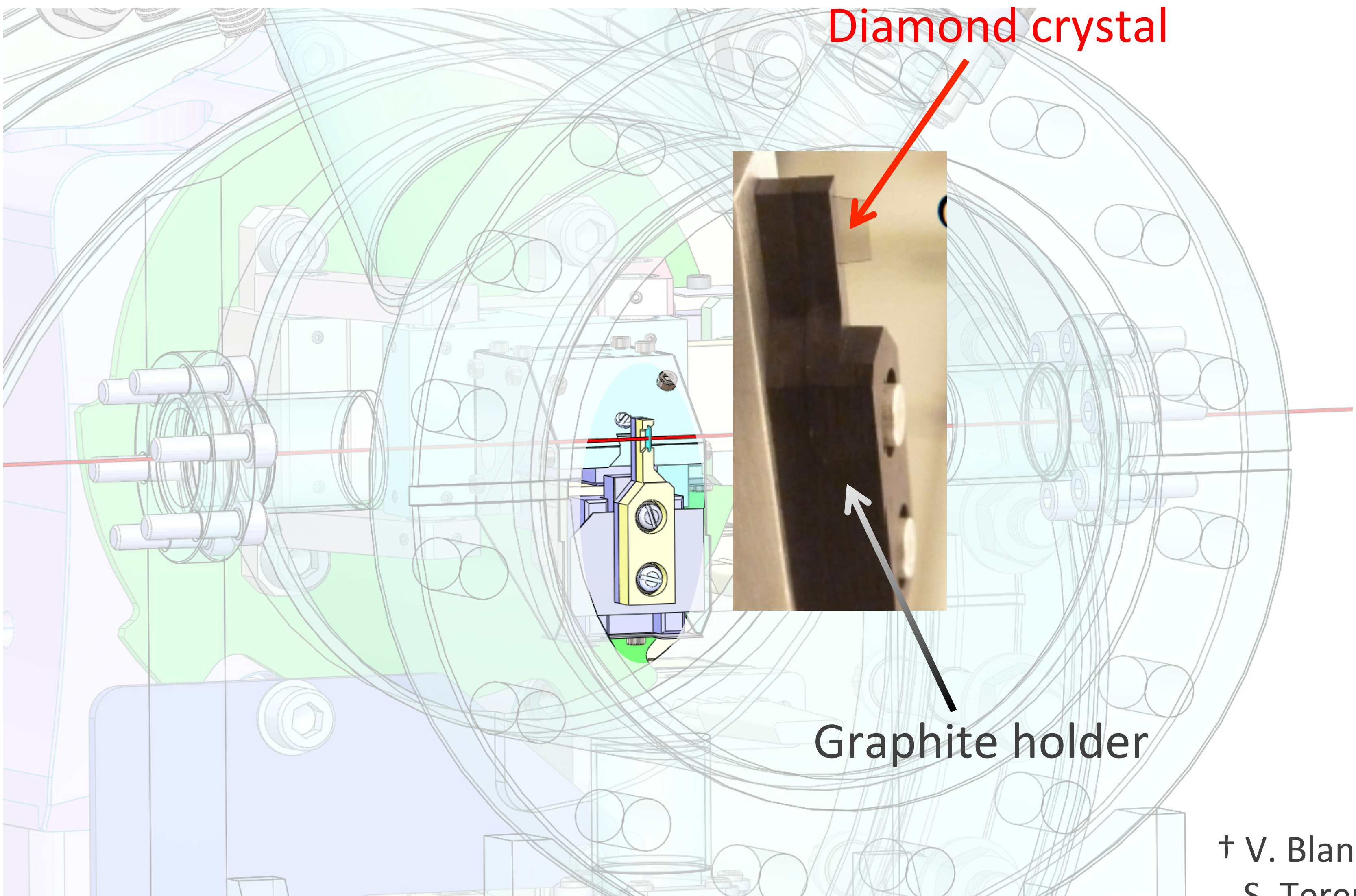


Diamond holder and positioning system



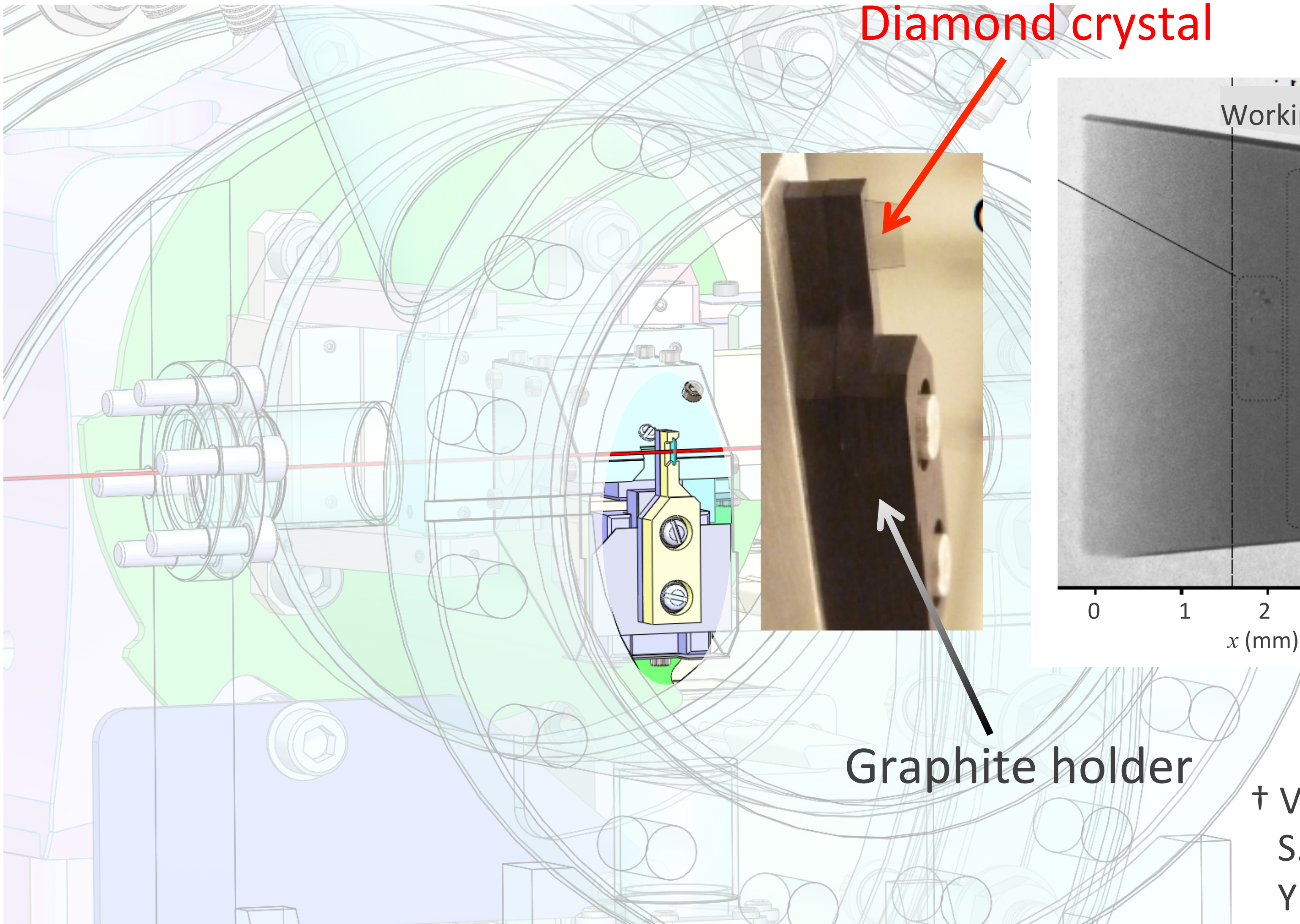
† D. Shu

Diamond holder and positioning system



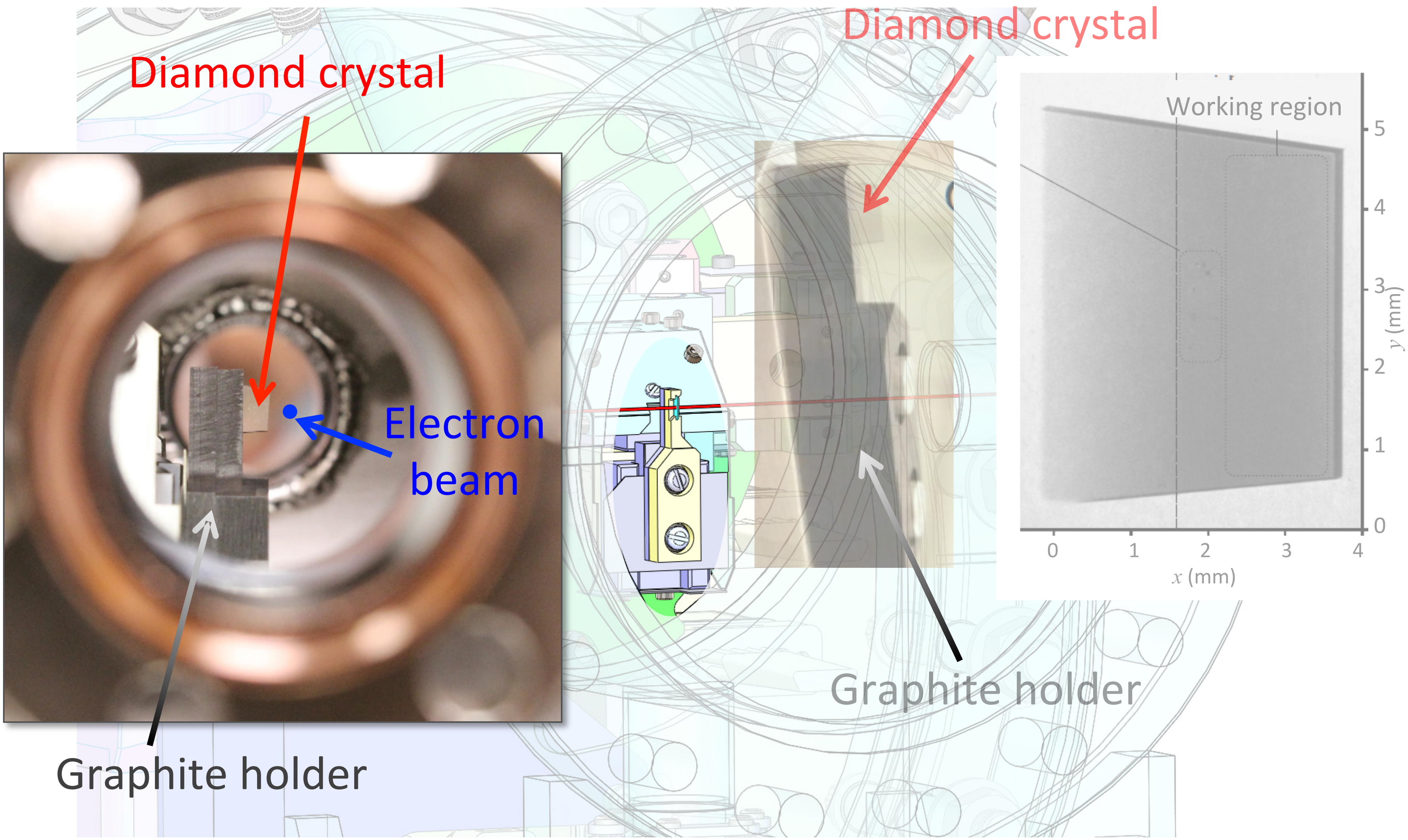
† V. Blank and S. Terentiev

Diamond holder and positioning system

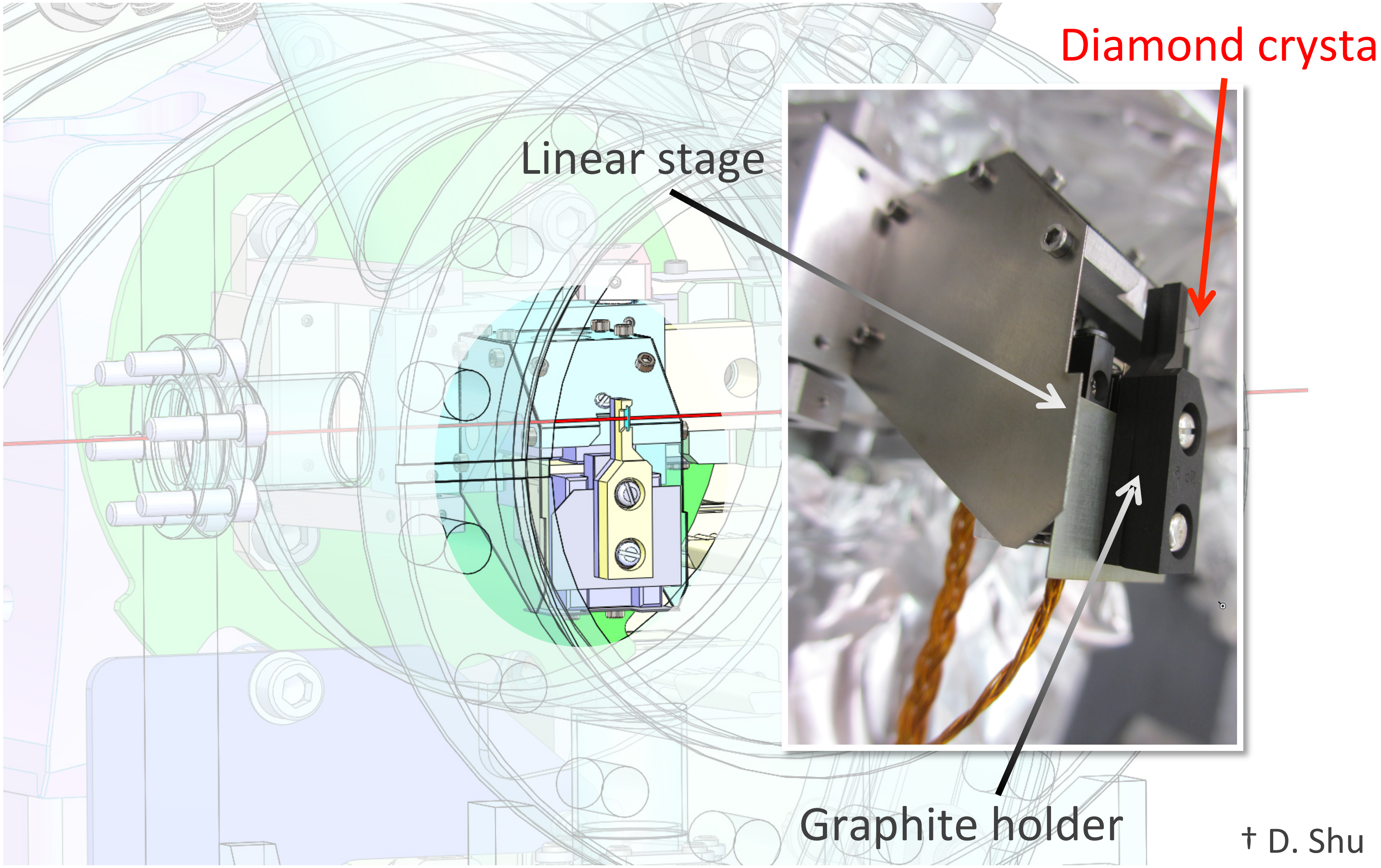


† V. Blank,
S. Terentiev,
Yu. Shvyd'ko
S. Stoupin,

Diamond holder and positioning system

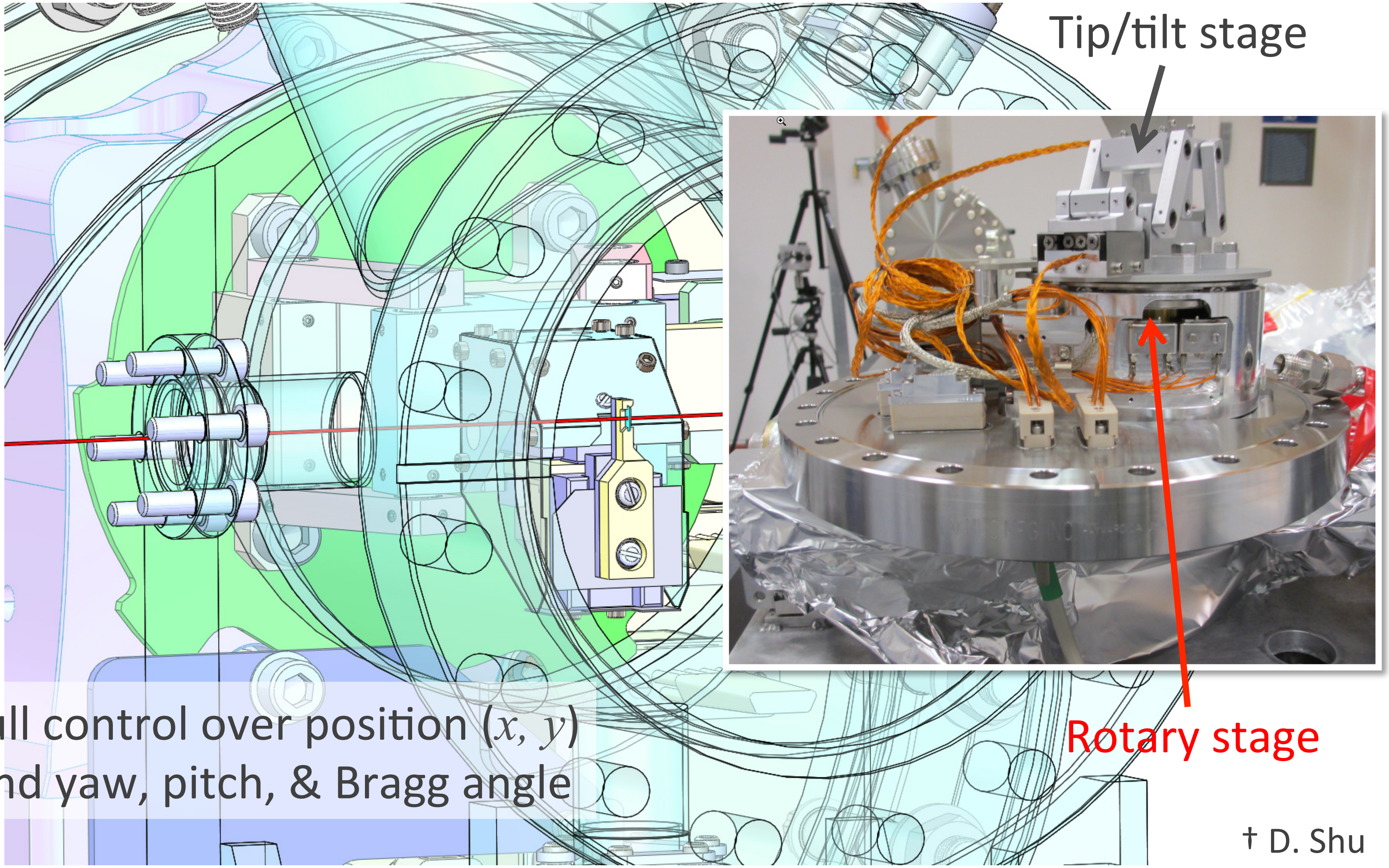


Diamond holder and positioning system



† D. Shu

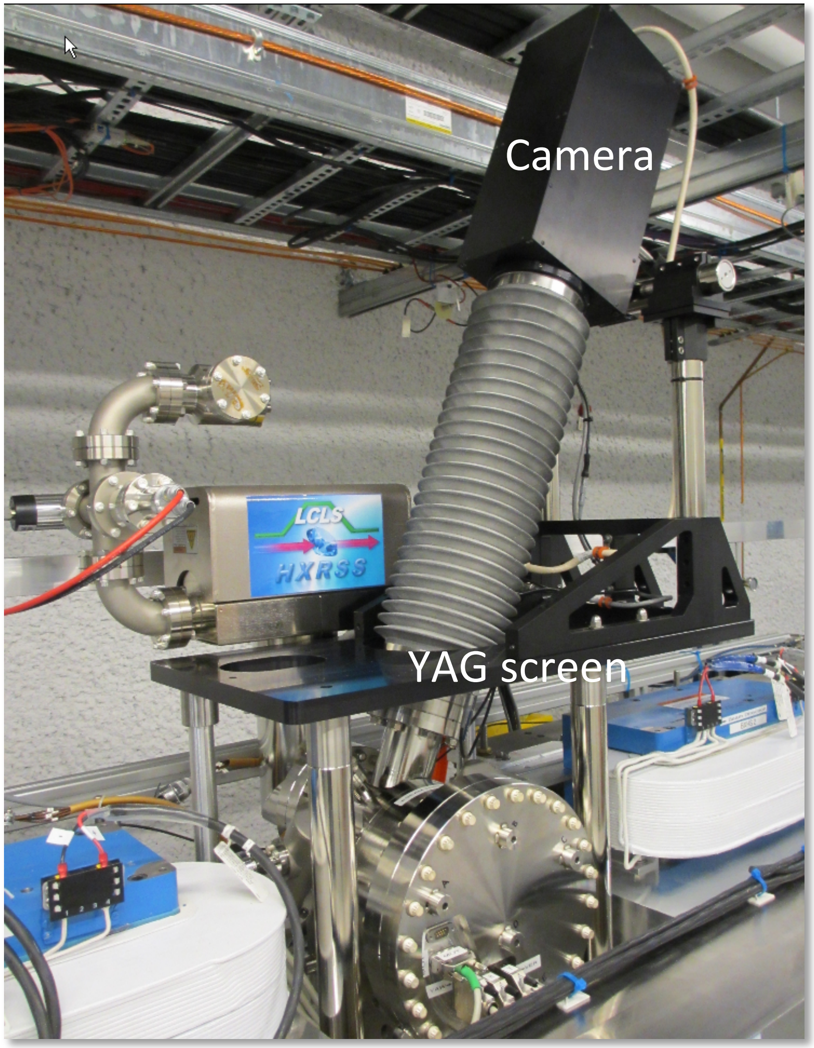
Diamond holder and positioning system

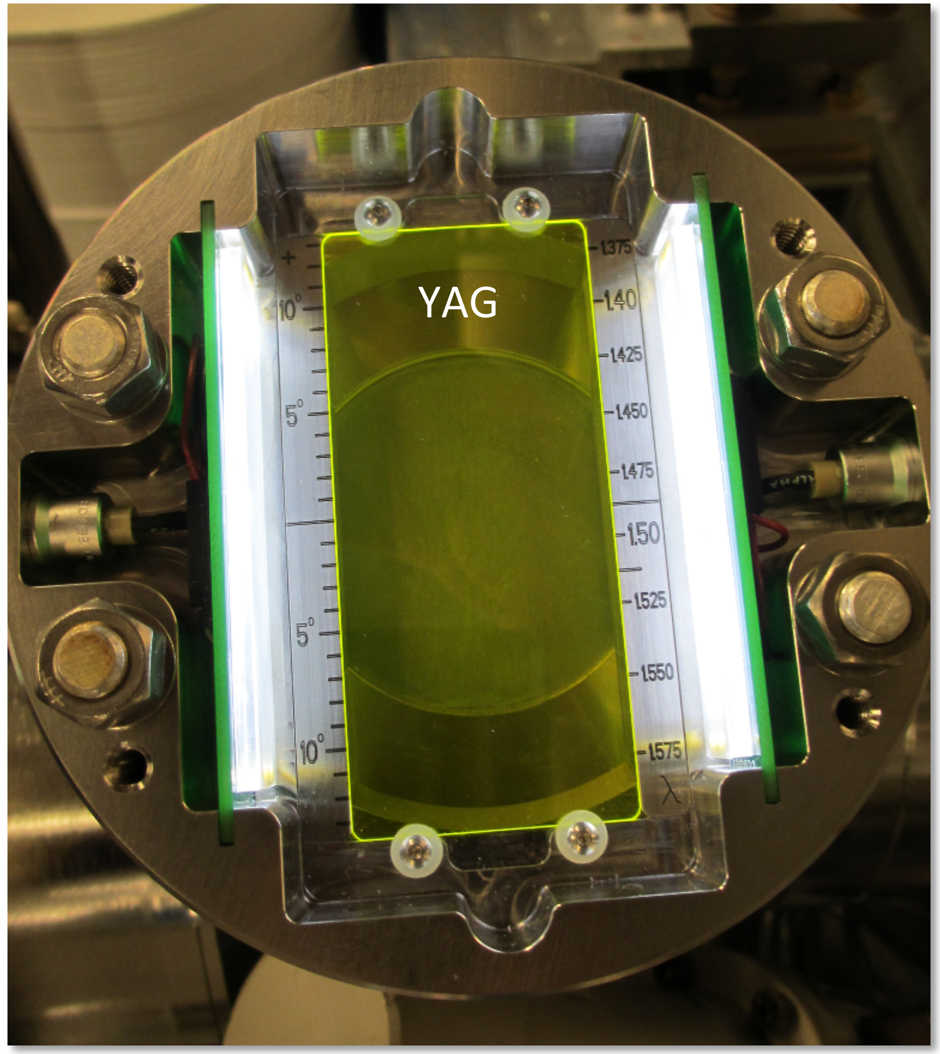


Full control over position (x, y) and yaw, pitch, & Bragg angle

† D. Shu

Bragg reflection diagnostic

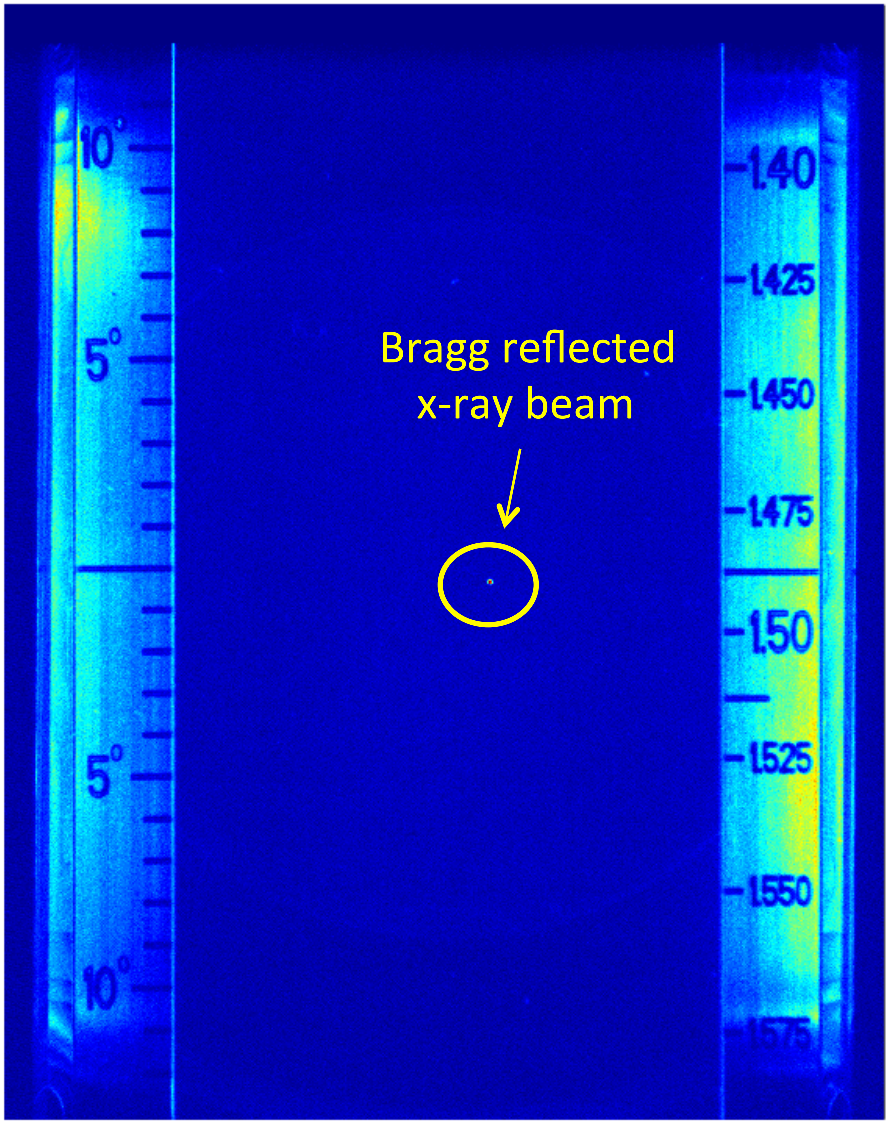




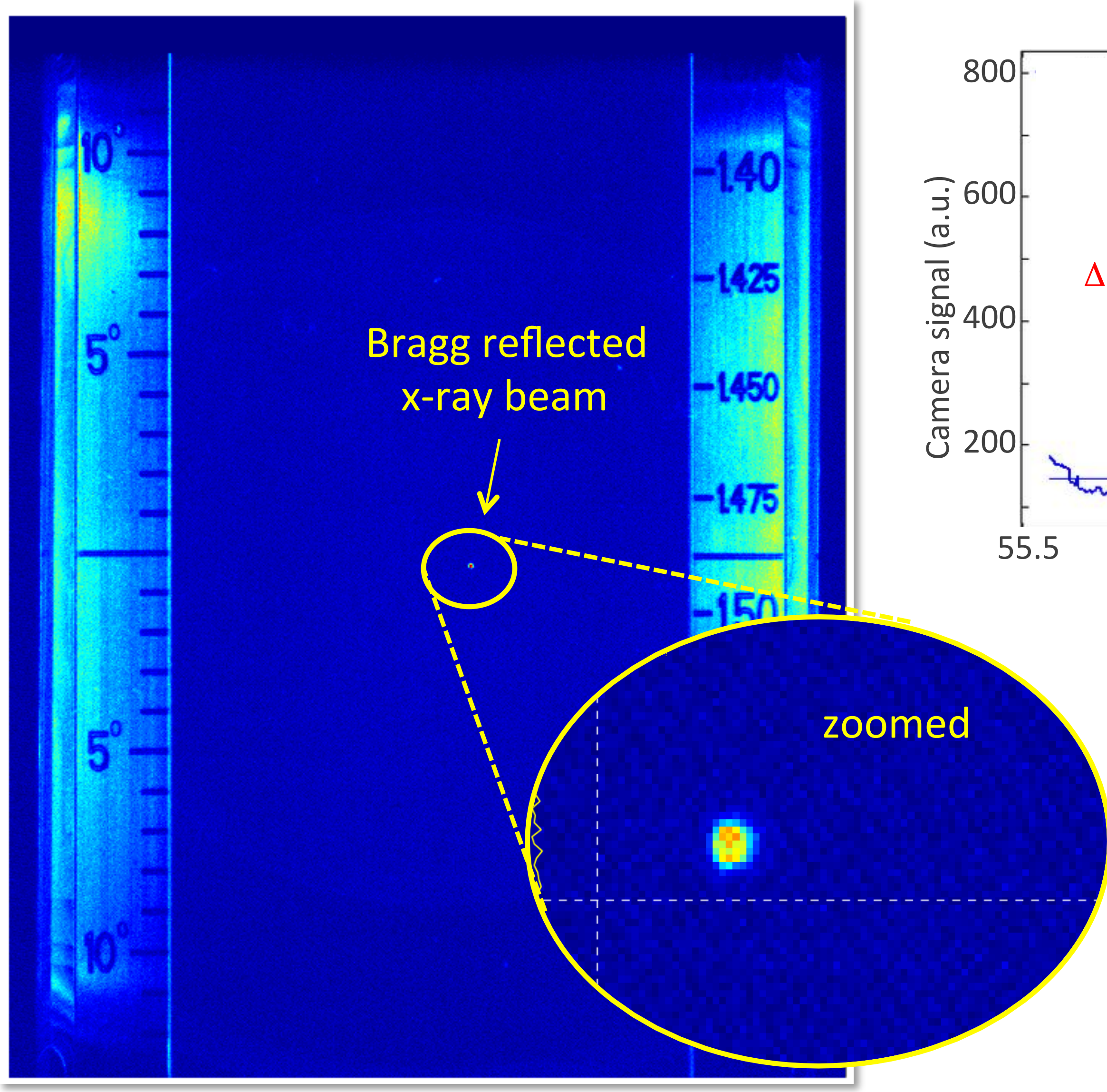
As suggested in G. Geloni, V. Kocharyan ,and E.L. Saldin, DESY 10-133, arXiv:1008.3036 (2010)

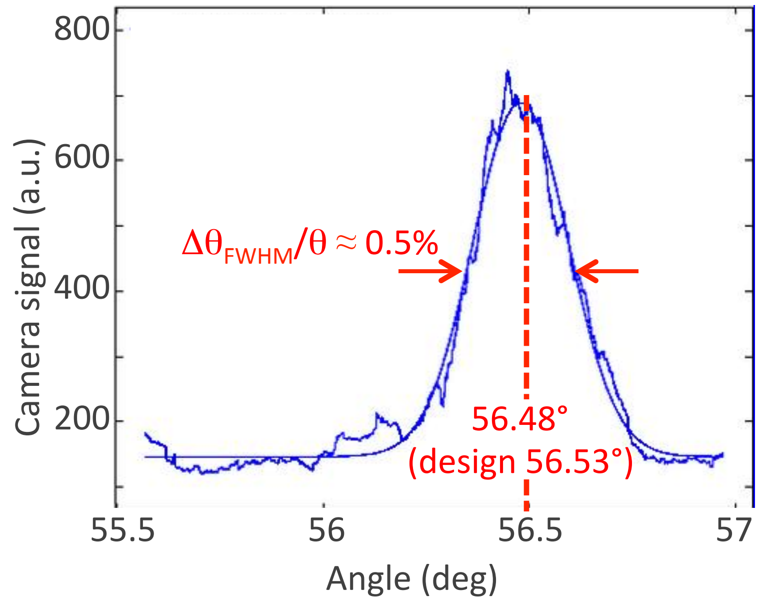
† B. Berg

First signal of successful mono operation

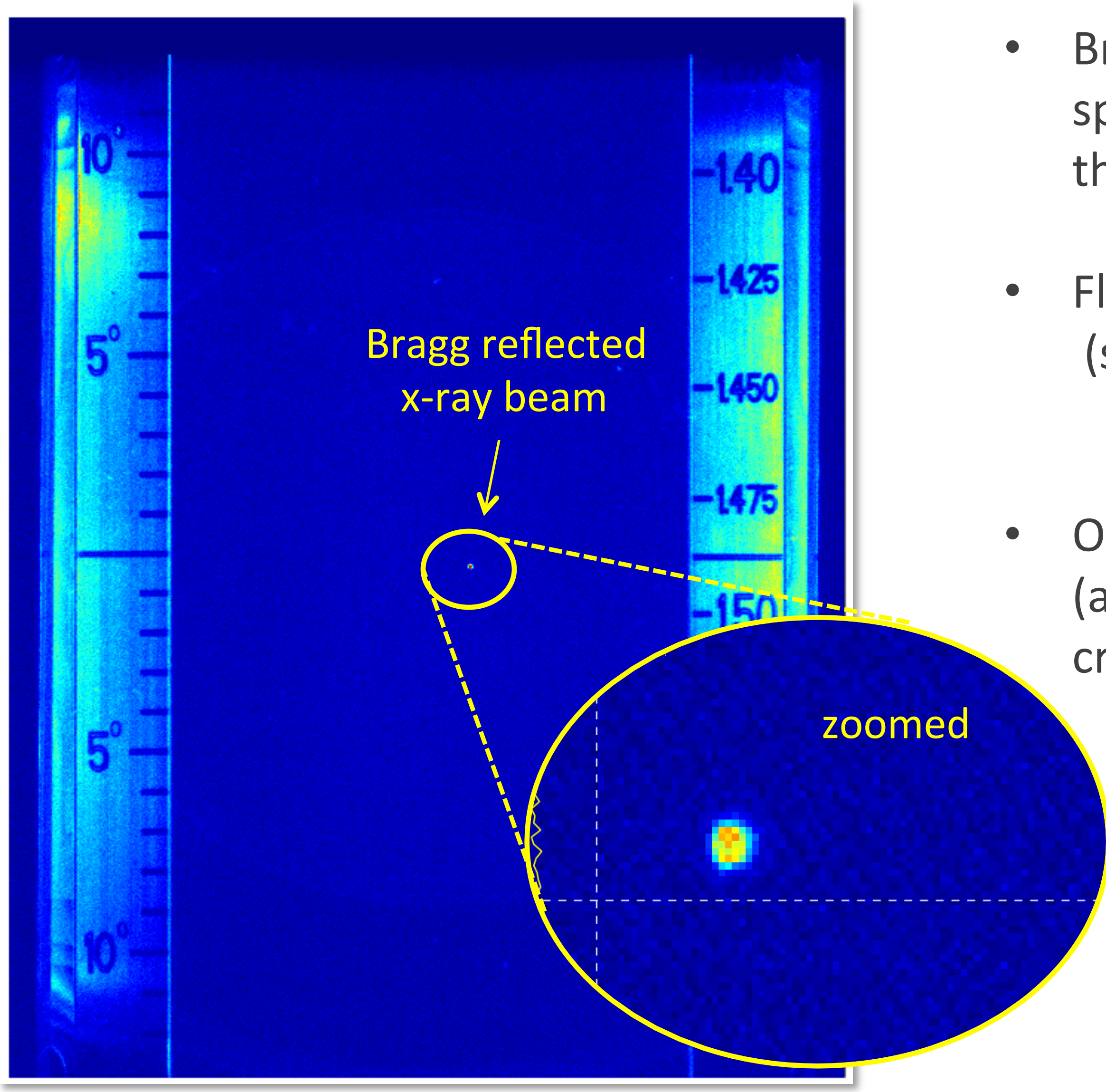


First signal of successful mono operation



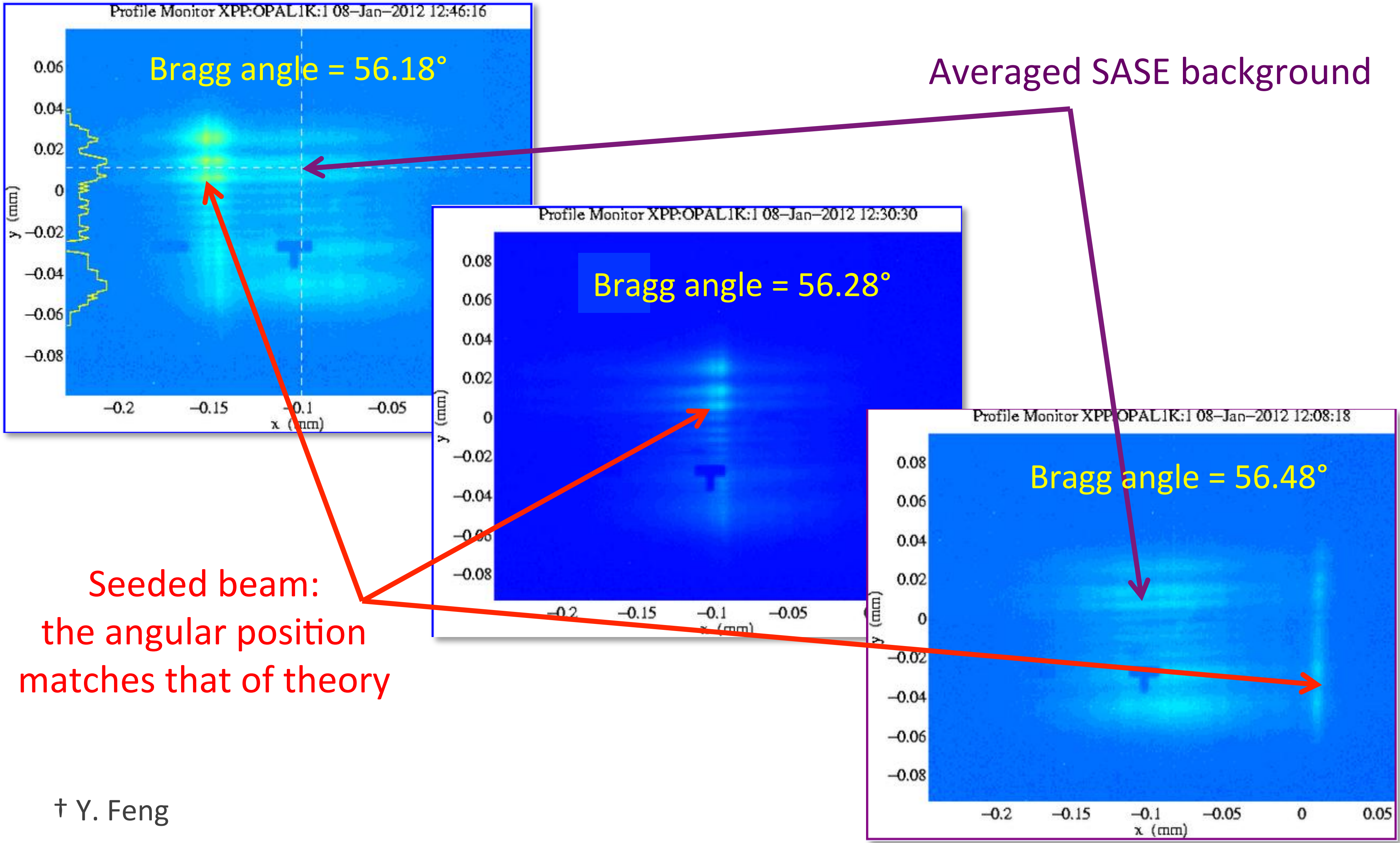


First signal of successful mono operation



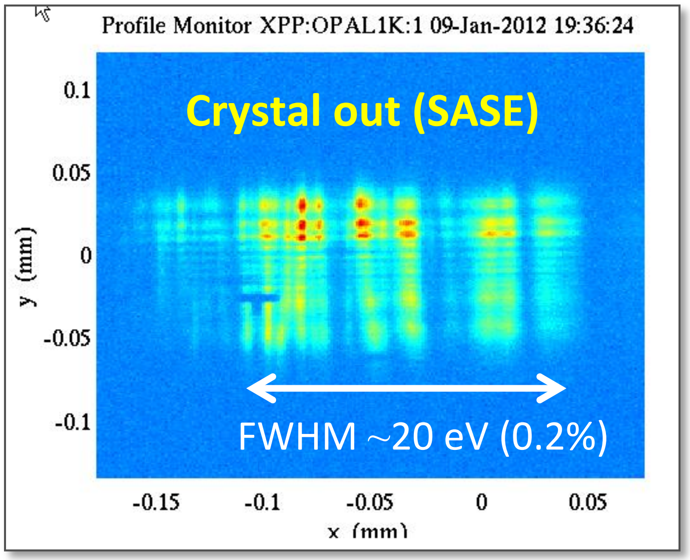
- Bragg reflected signal of spectral components in the transmission "notch"
- Fluctuations are 100% (single spectral mode before saturation)
- Of limited use for other (asymmetric or Laue) crystal reflections

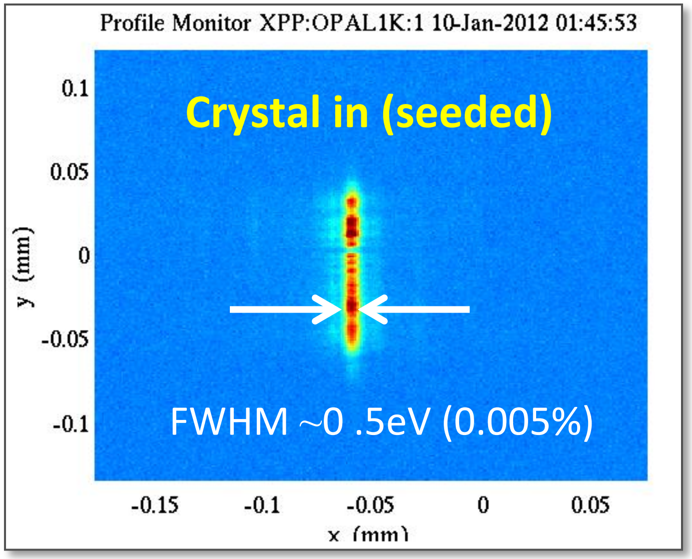
First indications of seeding from averaged spectra



† Y. Feng

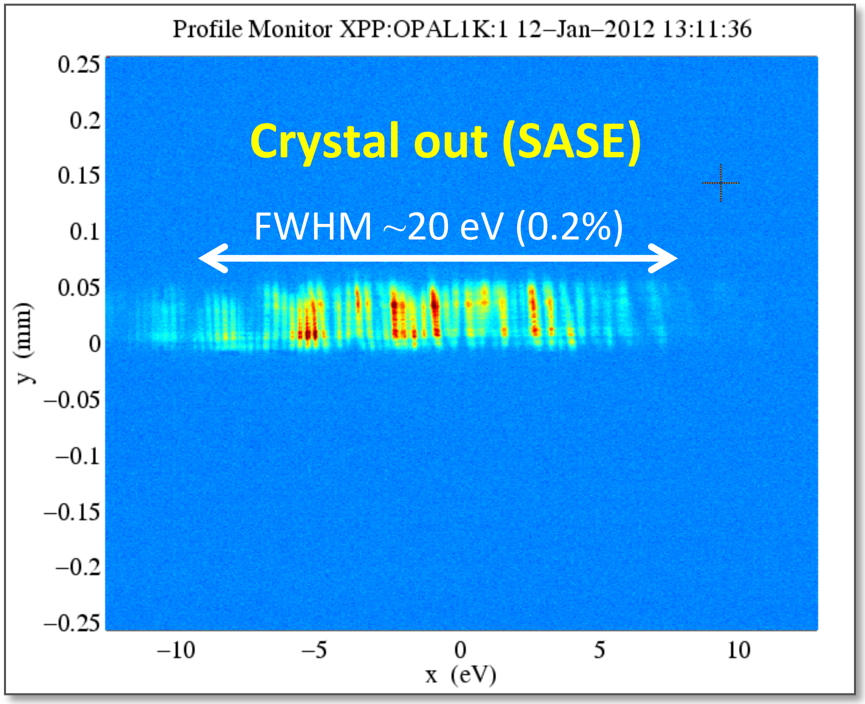
Slow improvements in power of seeded signal

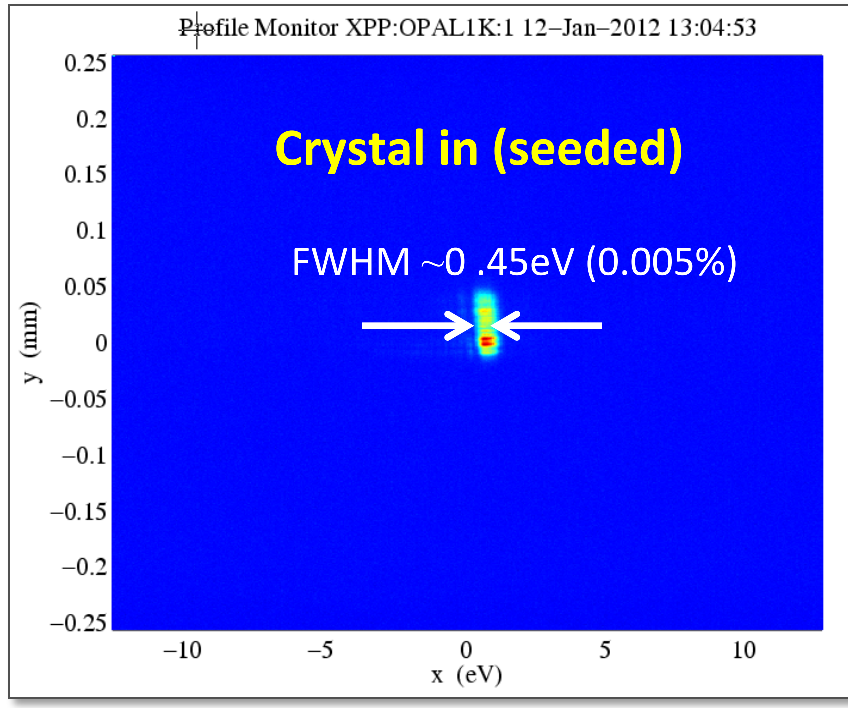




† Y. Feng

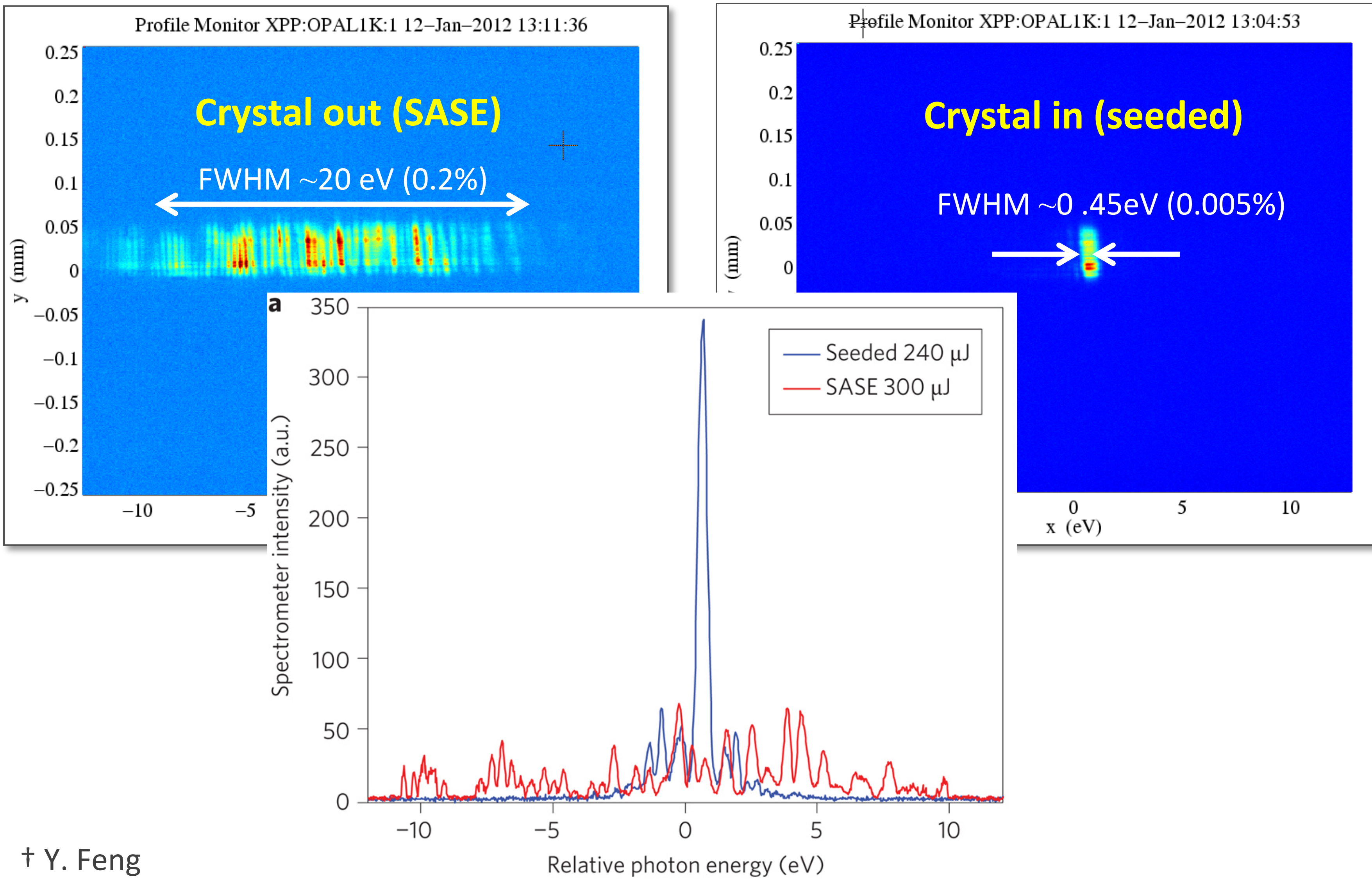
Slow improvements in power of seeded signal





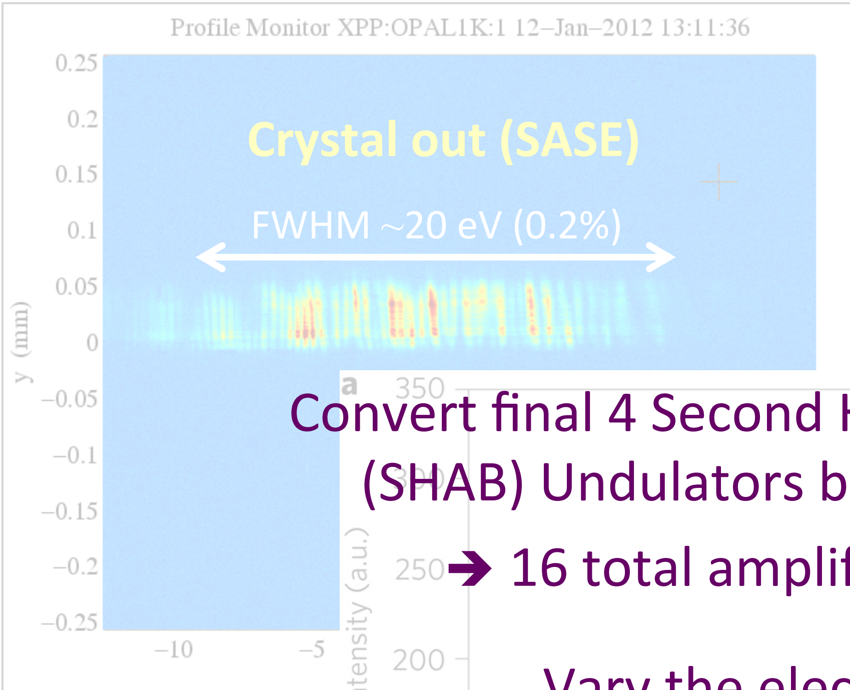
† Y. Feng

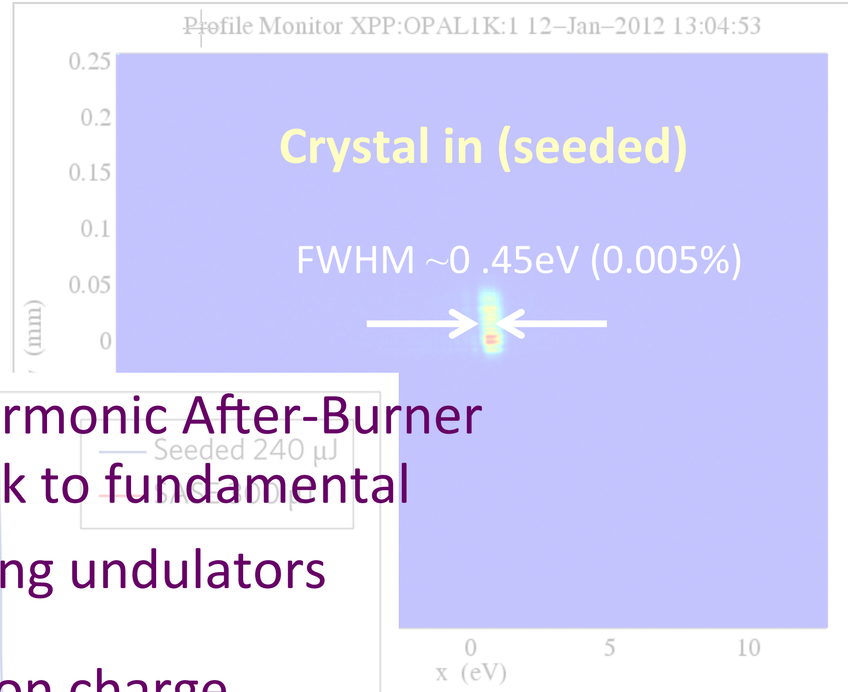
Slow improvements in power of seeded signal

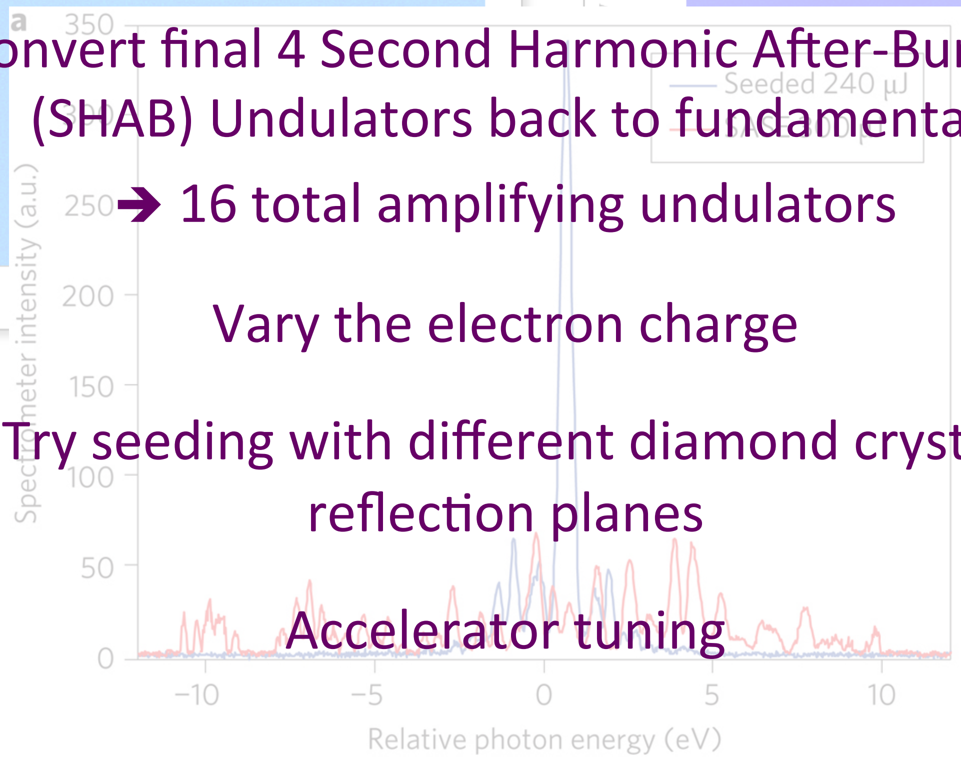


† Y. Feng

Slow improvements in power and stability







Convert final 4 Second Harmonic After-Burner (SHAB) Undulators back to fundamental

➔ 16 total amplifying undulators

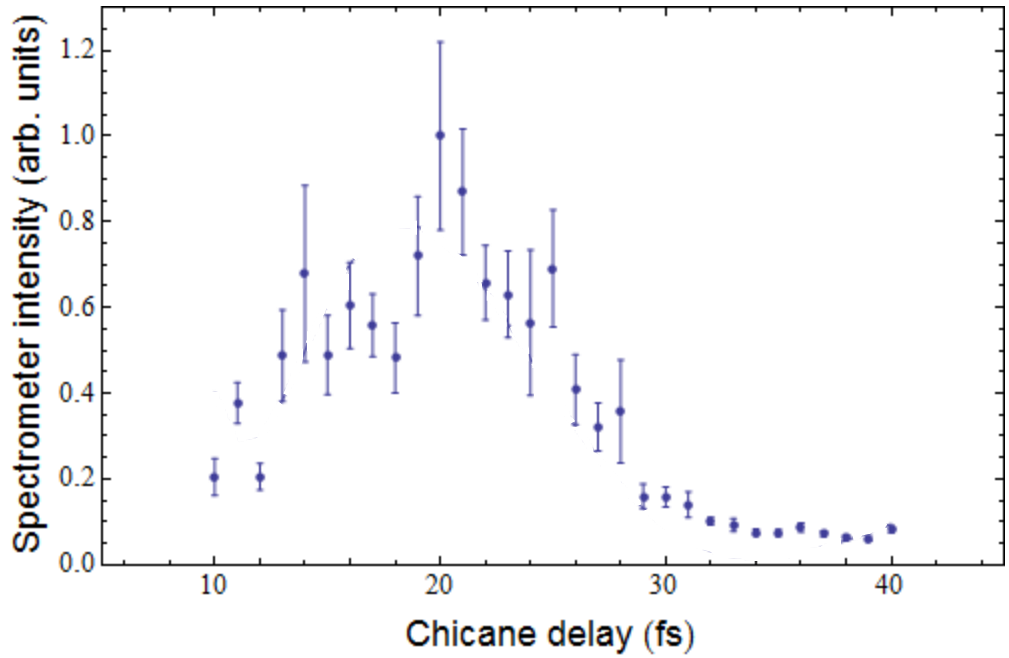
Vary the electron charge

Try seeding with different diamond crystal reflection planes

Accelerator tuning

Delay scan of seeding "wake"

Measure the seeded output as a function of the chicane time delay



Delay scan of seeding "wake"

Measure the seeded output as a function of the chicane time delay

Fit measurement to the predicted wake dependence using the dynamical theory of x-ray diffraction assuming:†

KNOWN: The time delay

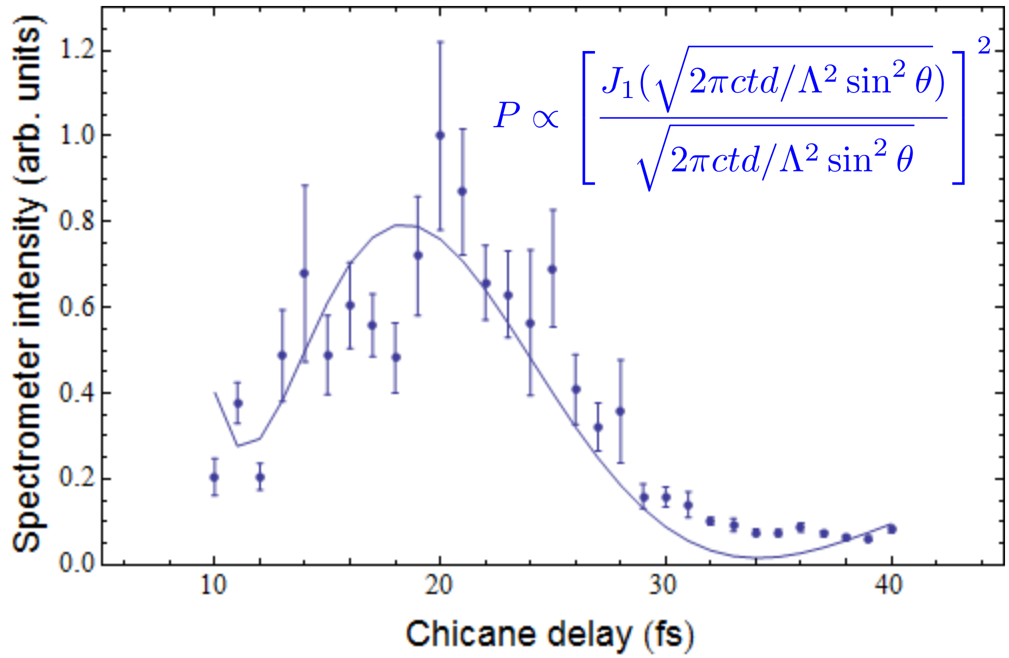
C(004) reflection

properties at 56.53°

FREE PARAMETERS:

Crystal thickness d

SASE pulse profile



† A. Zholents

Delay scan of seeding "wake"

Measure the seeded output as a function of the chicane time delay

Fit measurement to the predicted wake dependence using the dynamical theory of x-ray diffraction assuming:†

KNOWN: The time delay

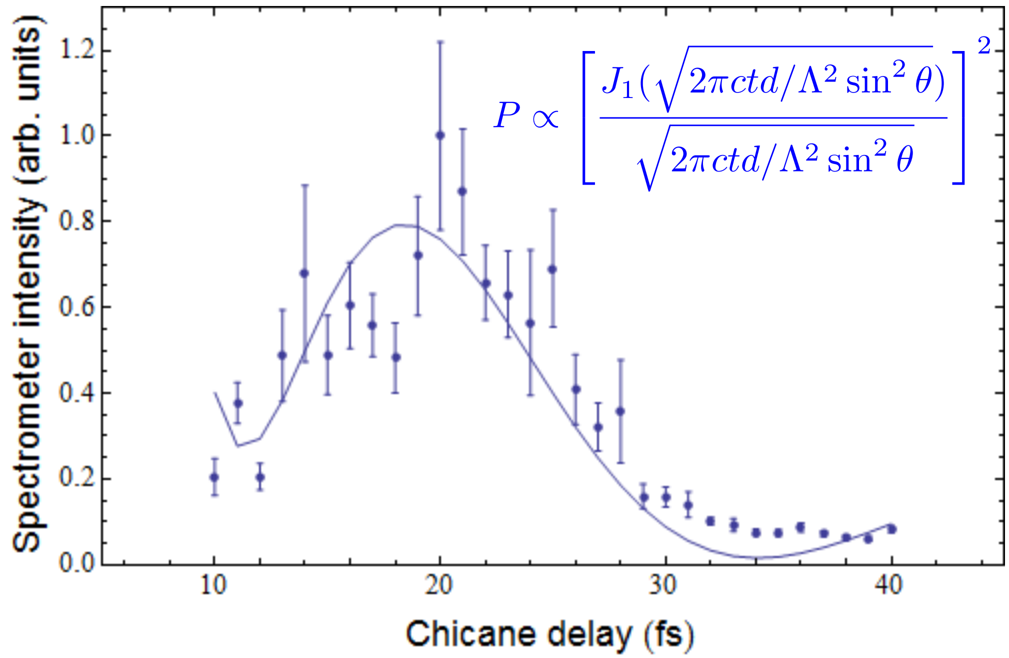
C(004) reflection properties at 56.53°

FREE PARAMETERS:

Crystal thickness d

SASE pulse profile

Best fit rather insensitive to beam shape; predicts crystal thickness equal to 104 microns and the SASE FWHM to be 3.5-5.5 fs



Pulse shape	d (μm)	T_{FWHM} (fs)
Flat-top	104	5.5
Gaussian	104	3.5
Parabolic	104	4.9

† A. Zholents

Delay scan of seeding "wake"

Measure the seeded output as a function of the chicane time delay

Fit measurement to the predicted wake dependence using the dynamical theory of x-ray diffraction assuming:†

KNOWN: The time delay

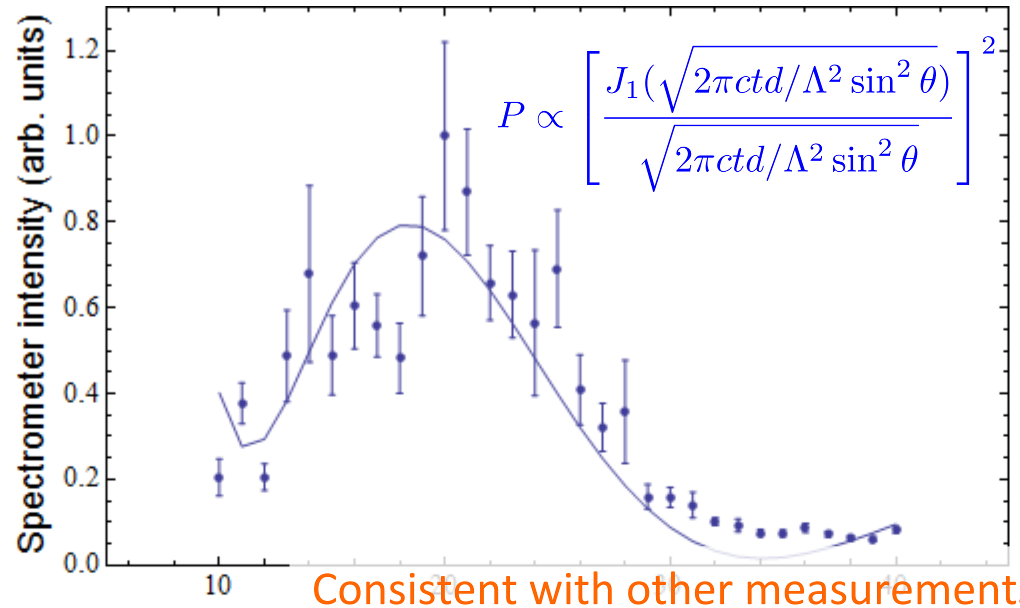
C(004) reflection properties at 56.53°

FREE PARAMETERS:

Crystal thickness d

SASE pulse profile

Best fit rather insensitive to beam shape; predicts crystal thickness equal to 104 microns and the SASE FWHM to be 3.5-5.5 fs



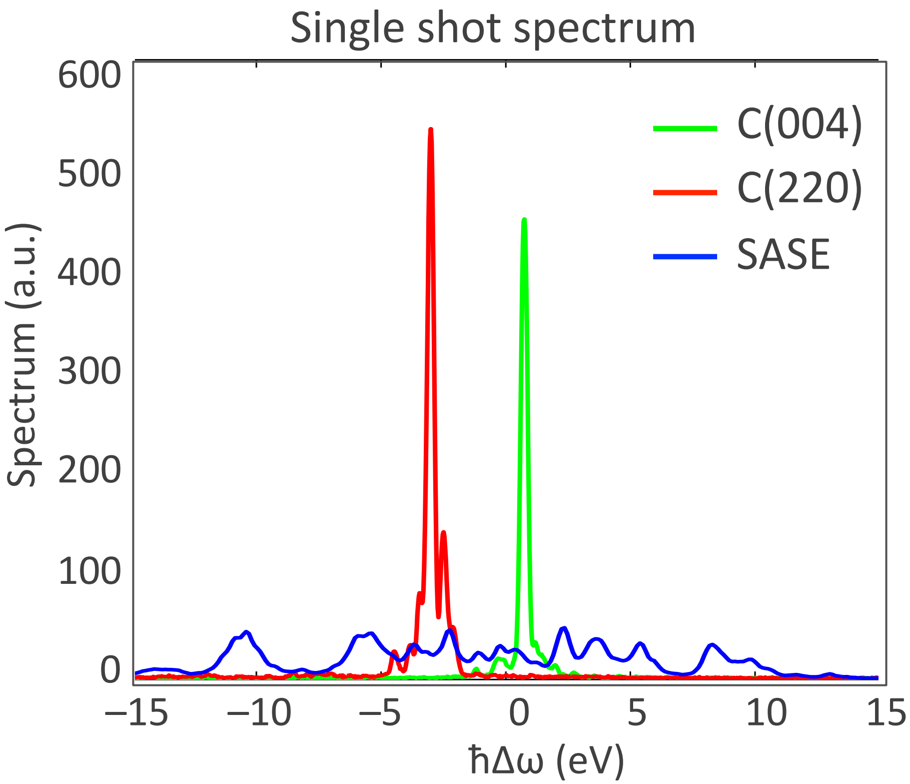
Consistent with other measurements (SASE correlation, e-beam length)

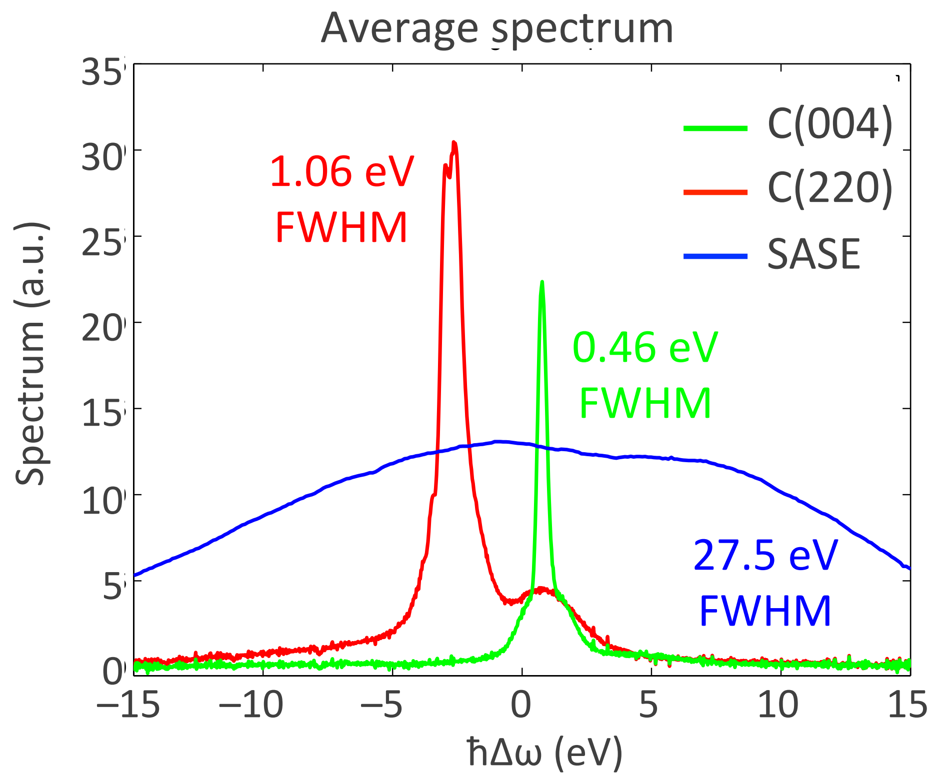
Pulse shape	d (µm)	T_{FWHM} (fs)
Flat-top	104	5.5
Gaussian	104	3.5
Parabolic	104	4.9

Agrees with measurements made at TISCNM

† A. Zholents

FEL spectra at 40 pC





Single shot bandwidth reduction by a factor ~ 50

Averaged bandwidth reduction ~ 25 to 50 depending on crystal reflection (different acceptances leads to different tolerances to fluctuations)

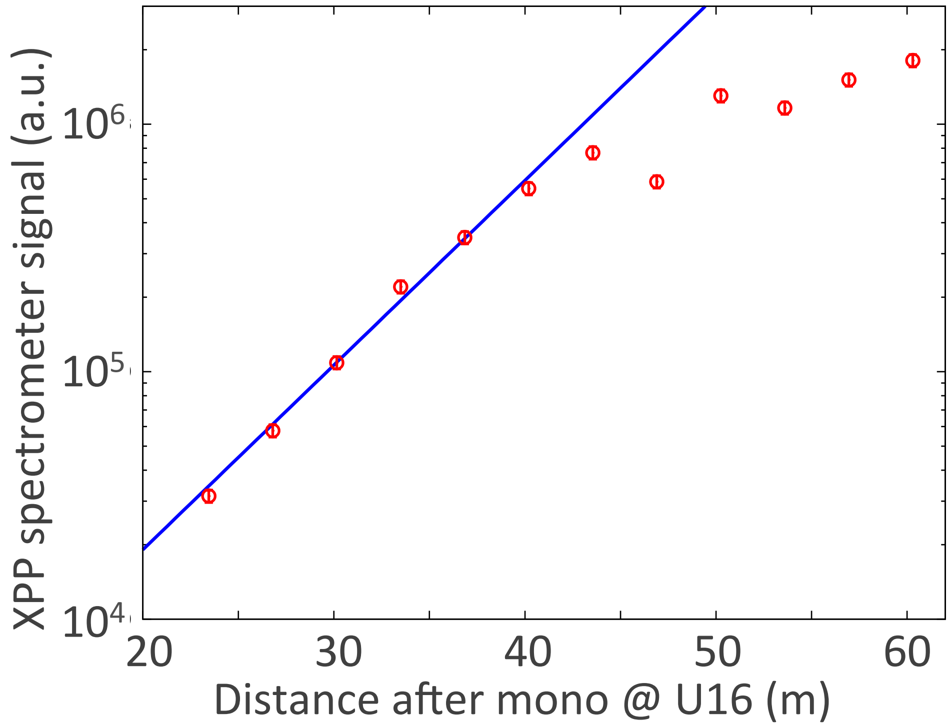
† A. Lutman

Gain and saturation of seeded signal

Using SASE produced by upstream Undulators 1-15 IN (None OUT)
plot power in downstream Undulators 17-33

$$L_G = 5.82 \pm 0.26 \text{ m}$$

$$P(z) \propto e^{6.4} \exp\left(\frac{z}{5.8 \text{ m}}\right)$$



† D. Ratner

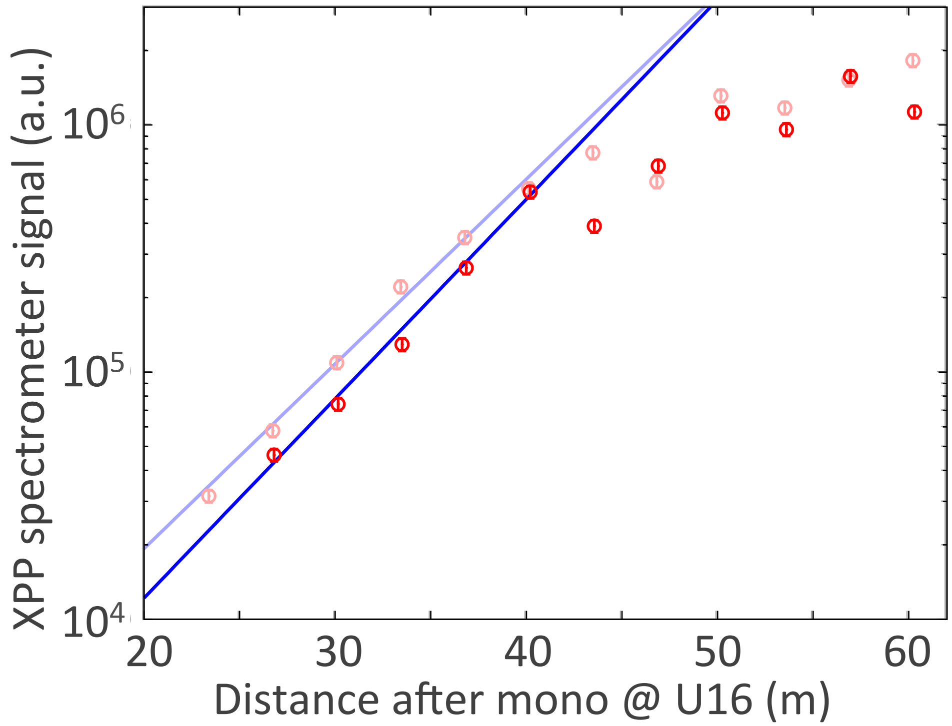
Gain and saturation of seeded signal

Using SASE produced by upstream Undulators 2-15 IN (One OUT)
plot power in downstream Undulators 17-33

$$P(z) \propto e^{6.4} \exp\left(\frac{z}{5.8\ \mathrm{m}}\right)$$

$$P(z) \propto e^{5.7} \exp\left(\frac{z}{5.4\ \mathrm{m}}\right)$$

$$L_G = 5.38 \pm 0.25\ \mathrm{m}$$



† D. Ratner

Gain and saturation of seeded signal

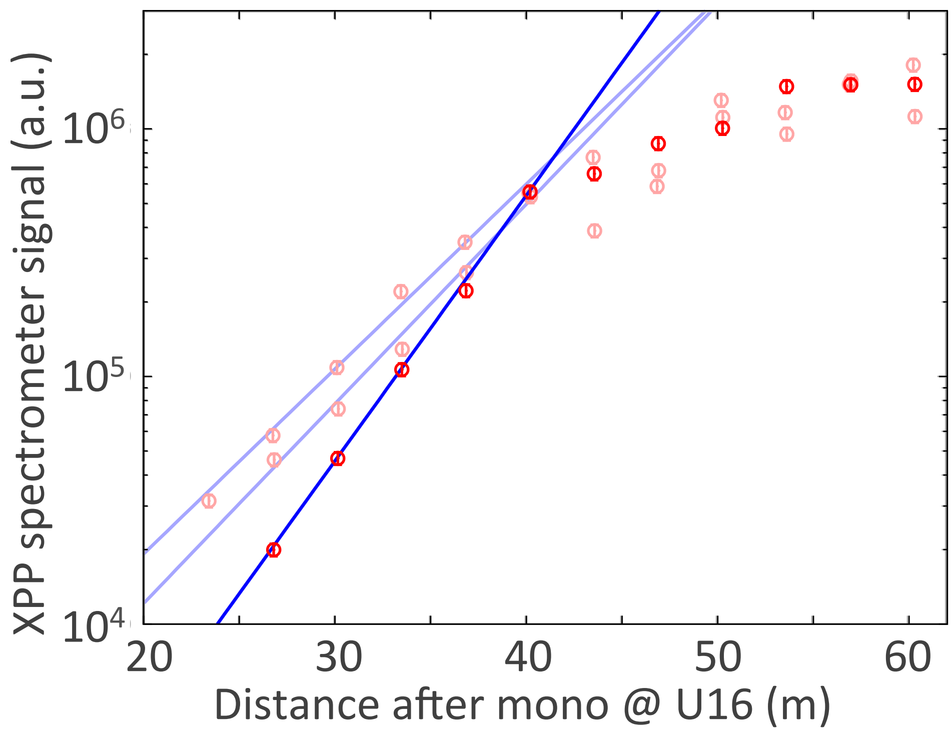
Using SASE produced by upstream Undulators 3-15 IN (Two OUT)
plot power in downstream Undulators 17-33

$$P(z) \propto e^{6.4} \exp\left(\frac{z}{5.8\ \mathrm{m}}\right)$$

$$P(z) \propto e^{5.7} \exp\left(\frac{z}{5.4\ \mathrm{m}}\right)$$

$$P(z) \propto e^{3.3} \exp\left(\frac{z}{4.1\ \mathrm{m}}\right)$$

$$L_G = 4.05 \pm 0.07\ \mathrm{m}$$

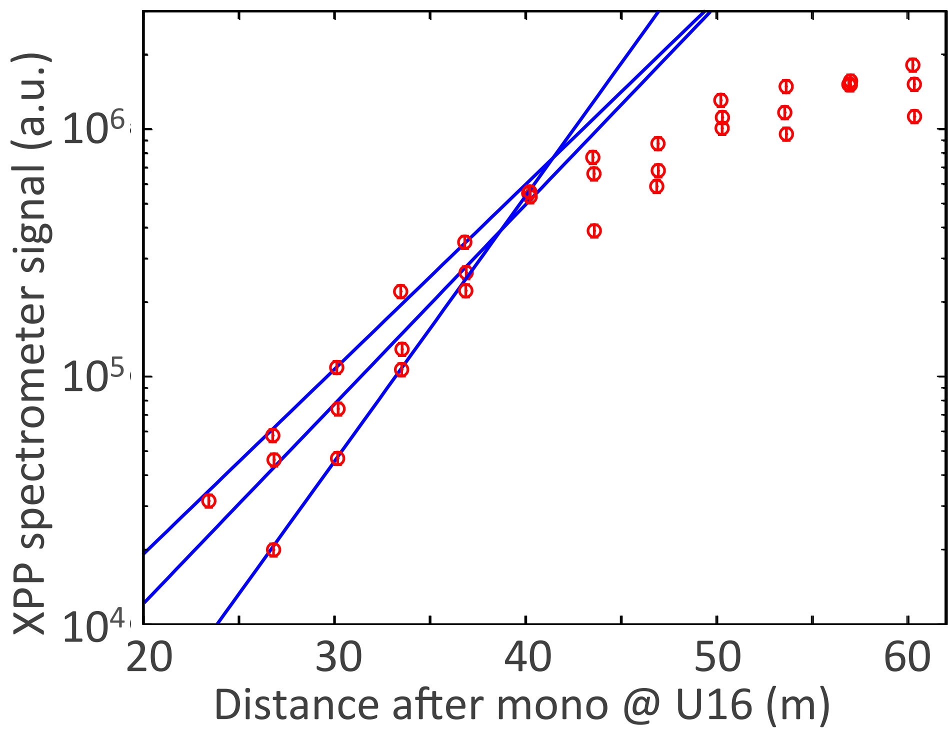


† D. Ratner

Gain and saturation of seeded signal

Ideally, one would like the SASE seeding undulator section to be ~14 gain lengths long to produce sufficient seeding power with minimal increase in energy spread

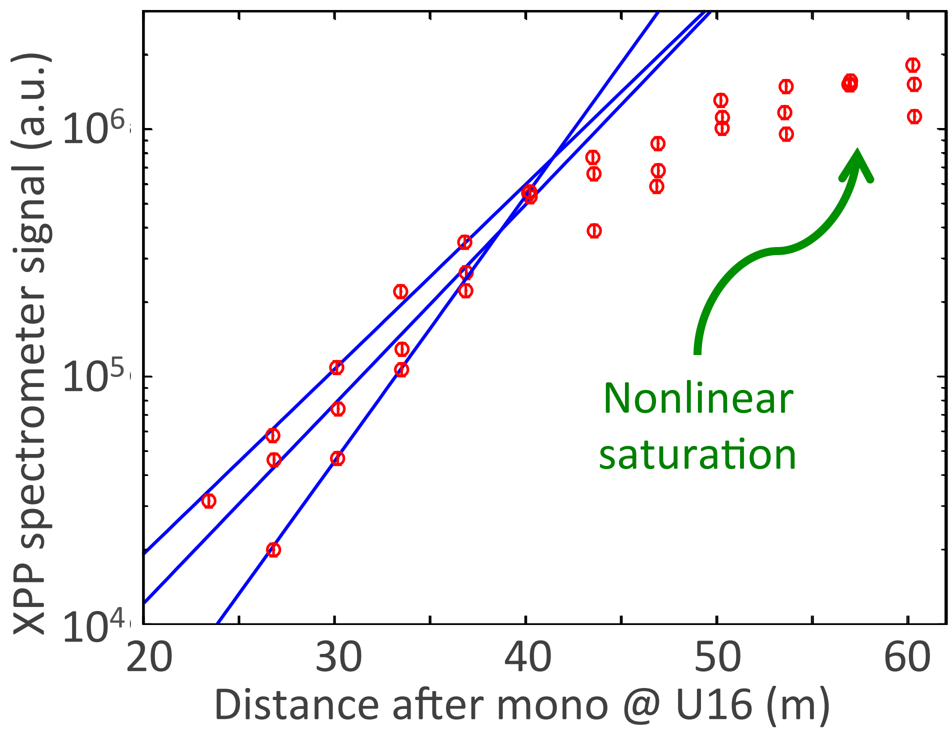
Optimal position of monochromator probably at Undulator 14 or 15 (depends on machine conditions, tuning)



Gain and saturation of seeded signal

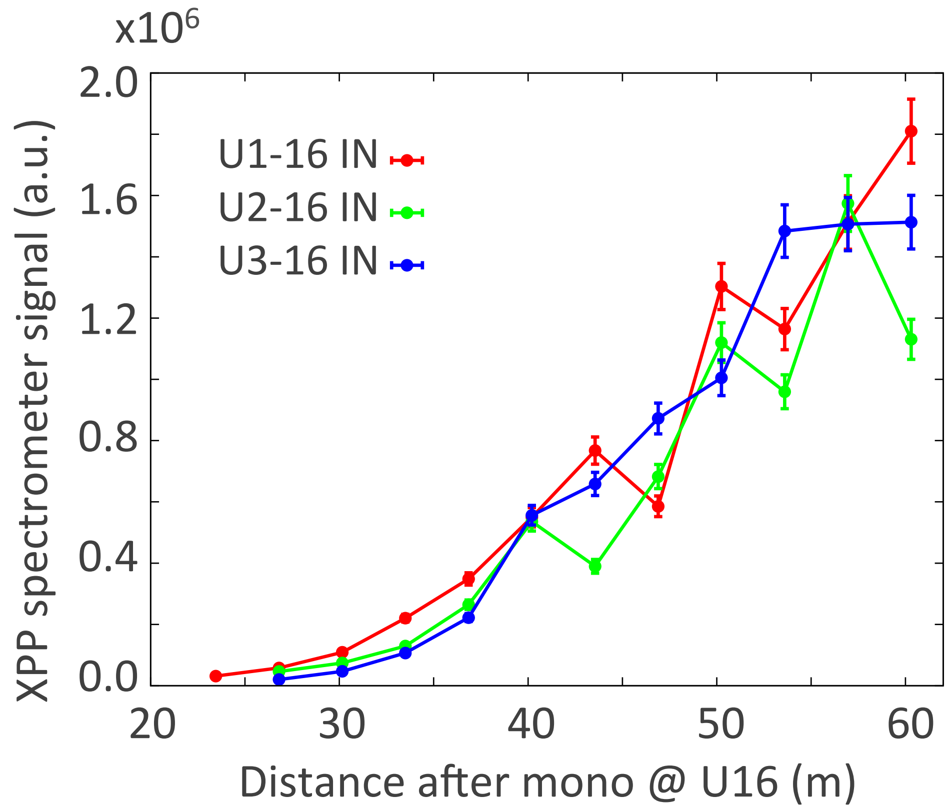
Ideally, one would like the SASE seeding undulator section to be ~14 gain lengths long to produce sufficient seeding power with minimal increase in energy spread

Optimal position of monochromator probably at Undulator 14 or 15 (depends on machine conditions, tuning)



"Soft" saturation with some evidence for oscillations in the power

- Synchrotron oscillations?
- Non-uniform amplification across the bunch? (i.e., the "current horns")?
- Other variations/ fluctuations?
- What does this mean for post saturation taper?

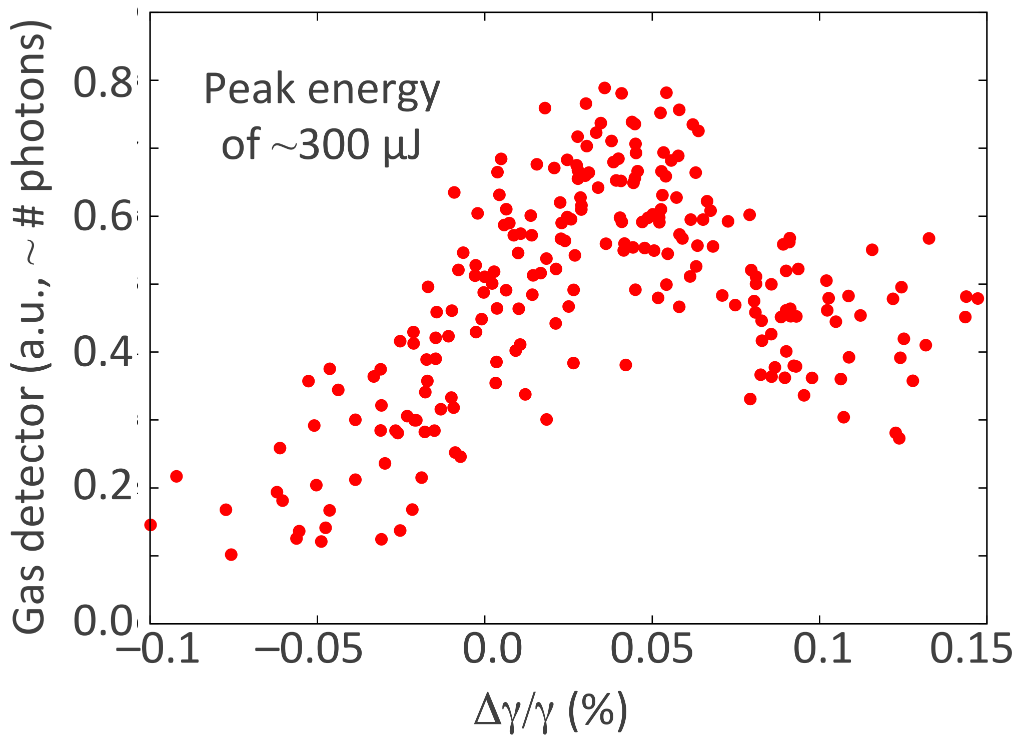


Energy in the seeded output

In addition to the usual requirements for SASE
(small emittance & energy spread, large peak current)
stable seeding requires precise control over
the longitudinal e-beam phase space

Energy in the seeded output

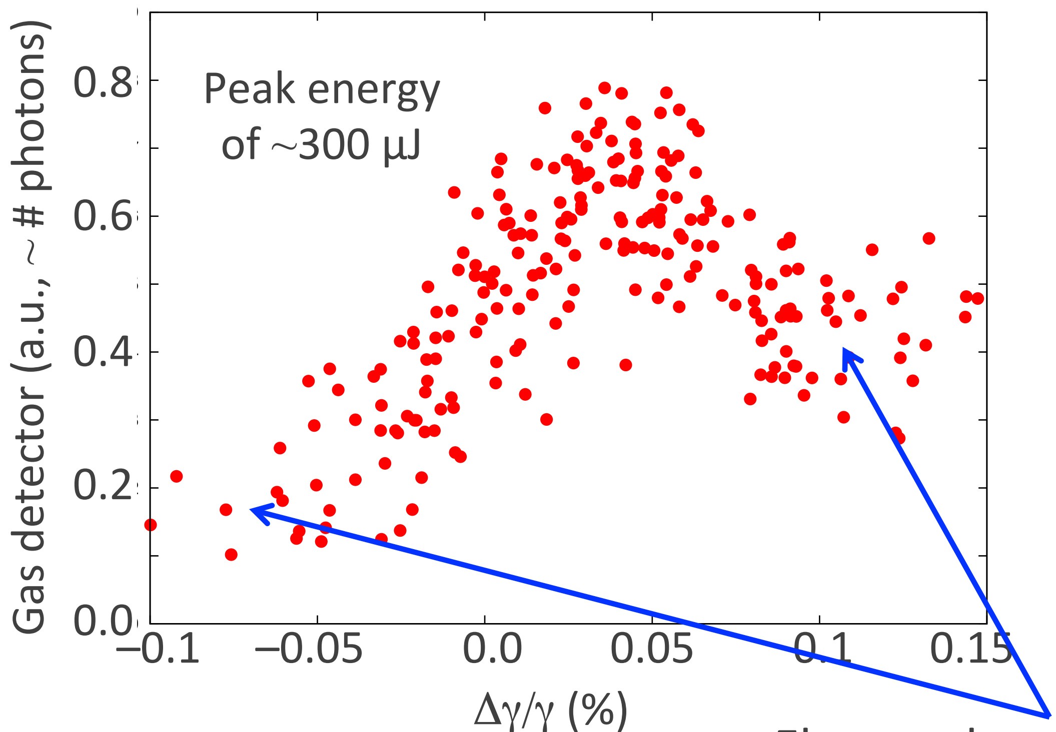
Jitter in mean e-beam energy maps onto variations in gain of seeded signal and thus in output photon number



† J. Welch, F.-J. Decker

Energy in the seeded output

Jitter in mean e-beam energy maps onto variations in gain of seeded signal and thus in output photon number

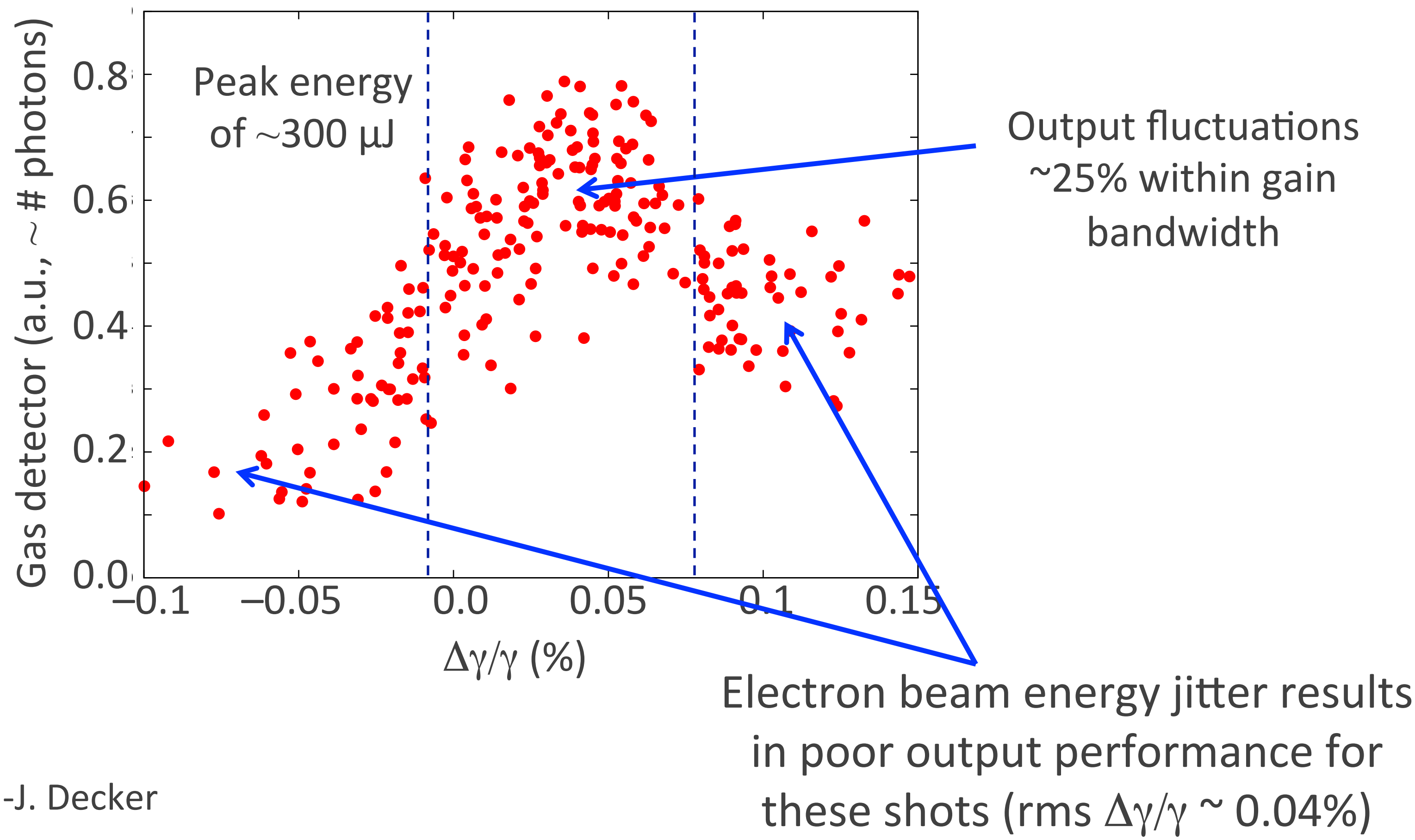


Electron beam energy jitter results in poor output performance for these shots (rms Δγ/γ ~ 0.04%)

† J. Welch, F.-J. Decker

Energy in the seeded output

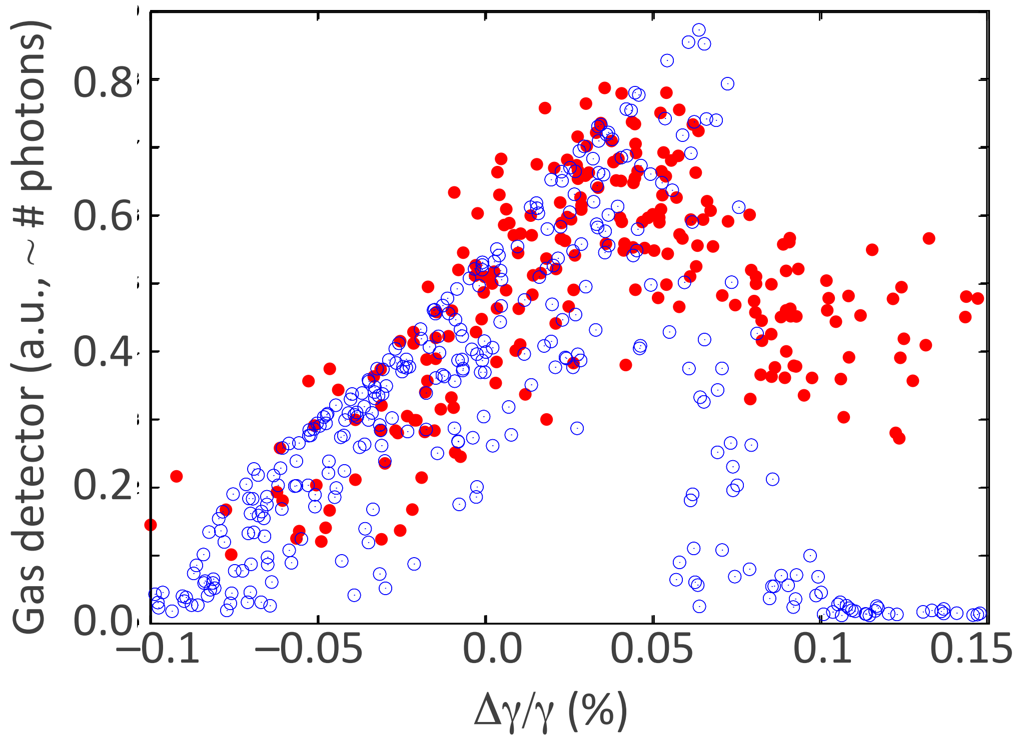
Jitter in mean e-beam energy maps onto variations in gain of seeded signal and thus in output photon number



† J. Welch, F.-J. Decker

Energy in the seeded output

Jitter in mean e-beam energy maps onto variations in gain of seeded signal and thus in output photon number

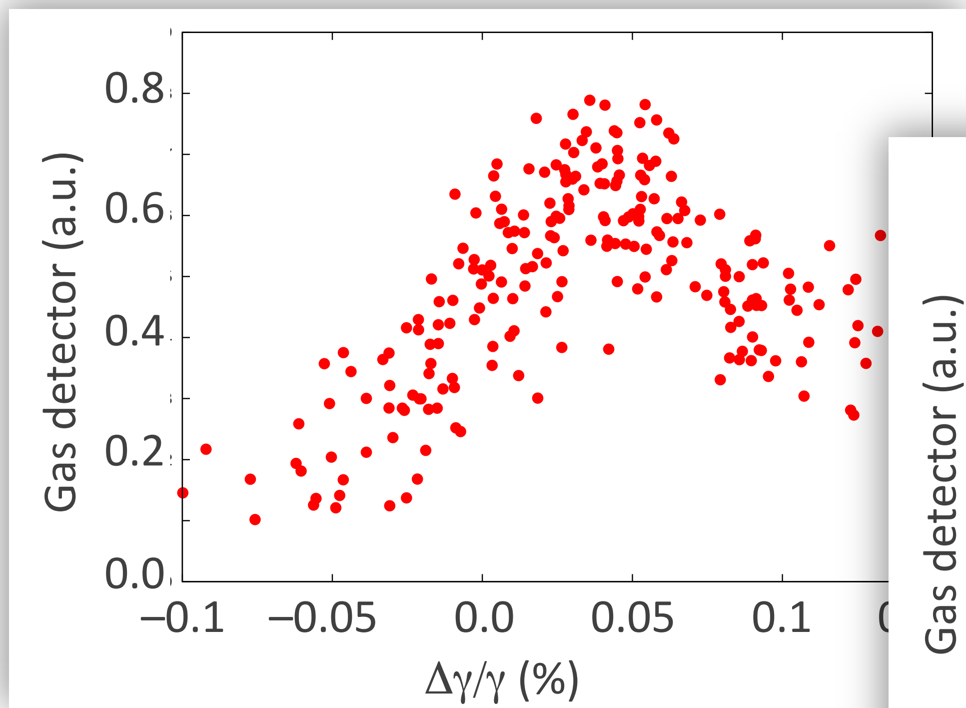


Compares reasonably well with simulations that reach saturation using $\rho \sim 6\text{x}10^{-4}$ and an rms energy jitter $\Delta\gamma/\gamma = 4\text{x}10^{-4}$

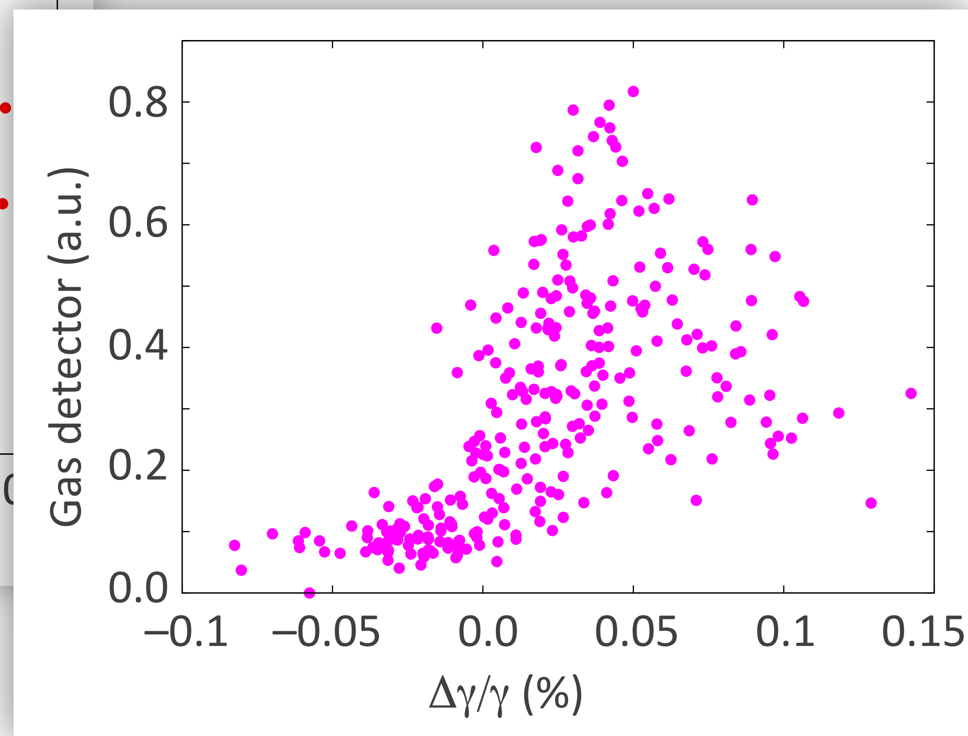
Energy in the seeded output

Depends strongly on machine parameters/tuning

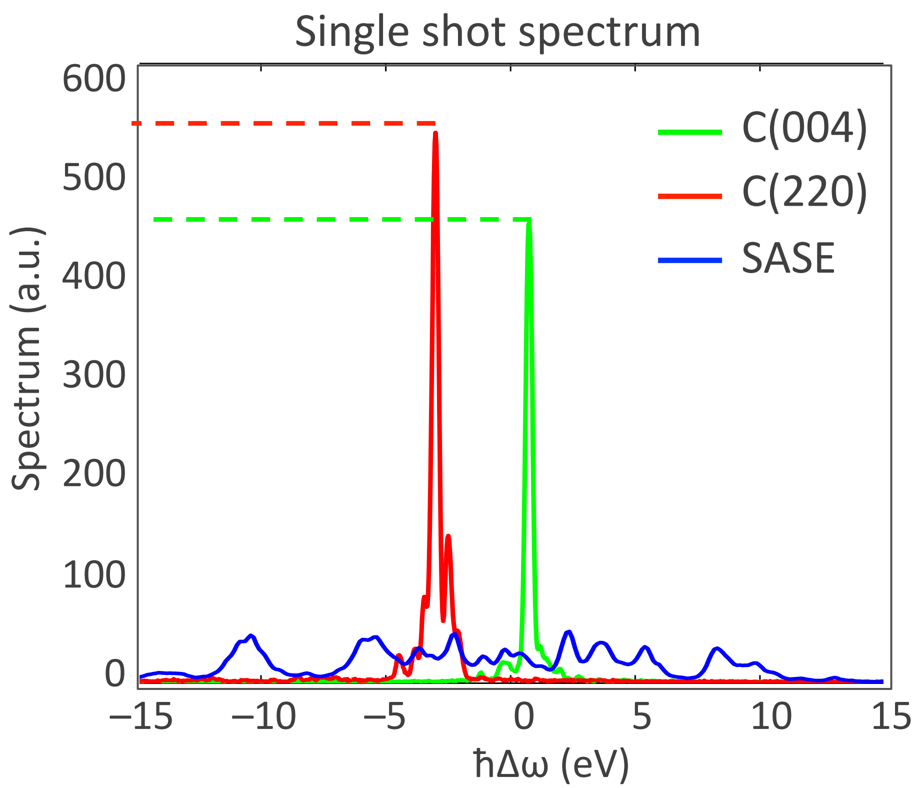
Output fluctuations ~25% within gain bandwidth

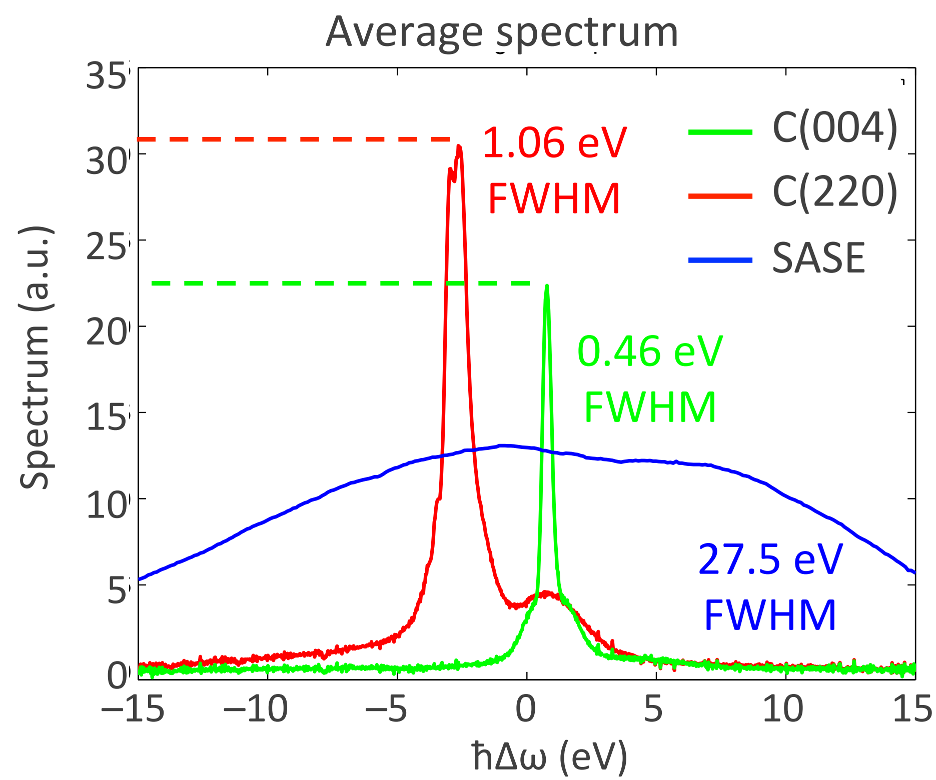


Output fluctuations ~50% within gain bandwidth



Fluctuations and spectral brightness for two diamond crystal reflections





Fluctuations reduce ensemble averaged seeded spectral brightness by a factor ≥ 18 from its peak value

BUT, seeded spectral brightness still larger than SASE

Depends on accelerator conditions, tuning

† A. Lutman

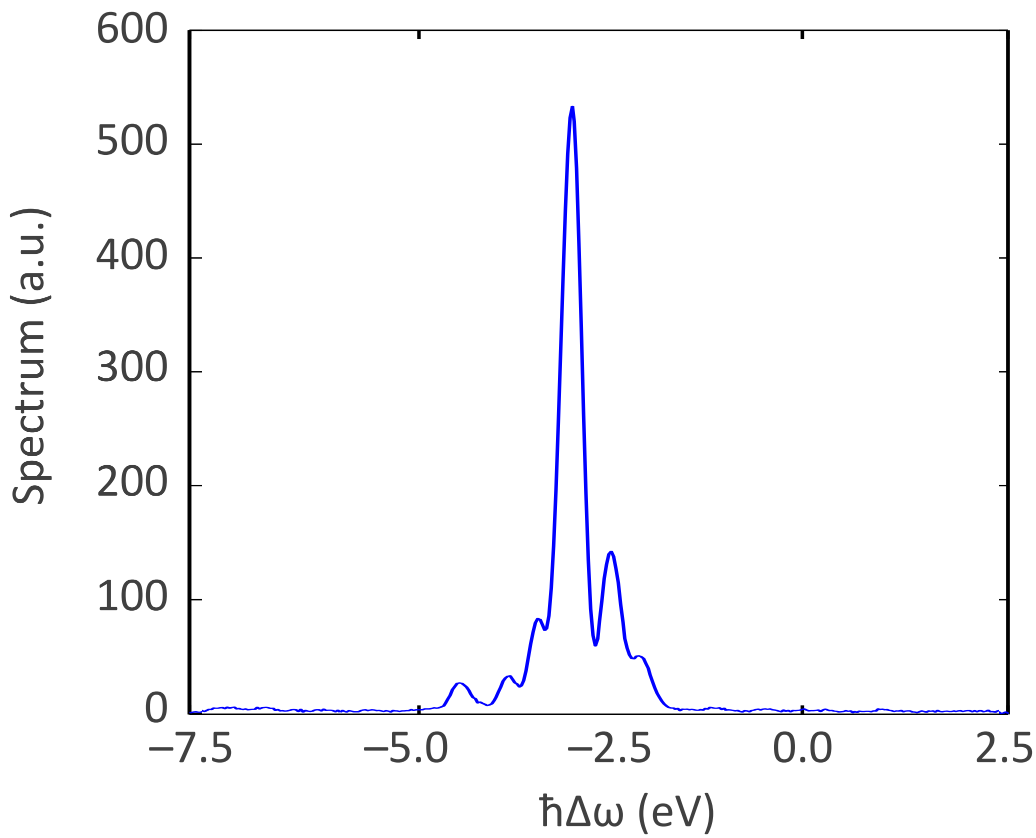
Other variations can be mapped onto spectrum

Variations in current?
("current horns")

Energy modulations?

Crystal vibrations?

???



† A. Lutman

Conclusions

- The wake monochromator concept can be experimentally realized
- Hard x-ray self-seeding has been implemented at the LCLS with a measured output bandwidth $\Delta\omega/\omega \sim 5\text{x}10^{-5}$ at 1.5 Å
- Clear signs of seeded saturation have been observed
- Fluctuations in output still somewhat high

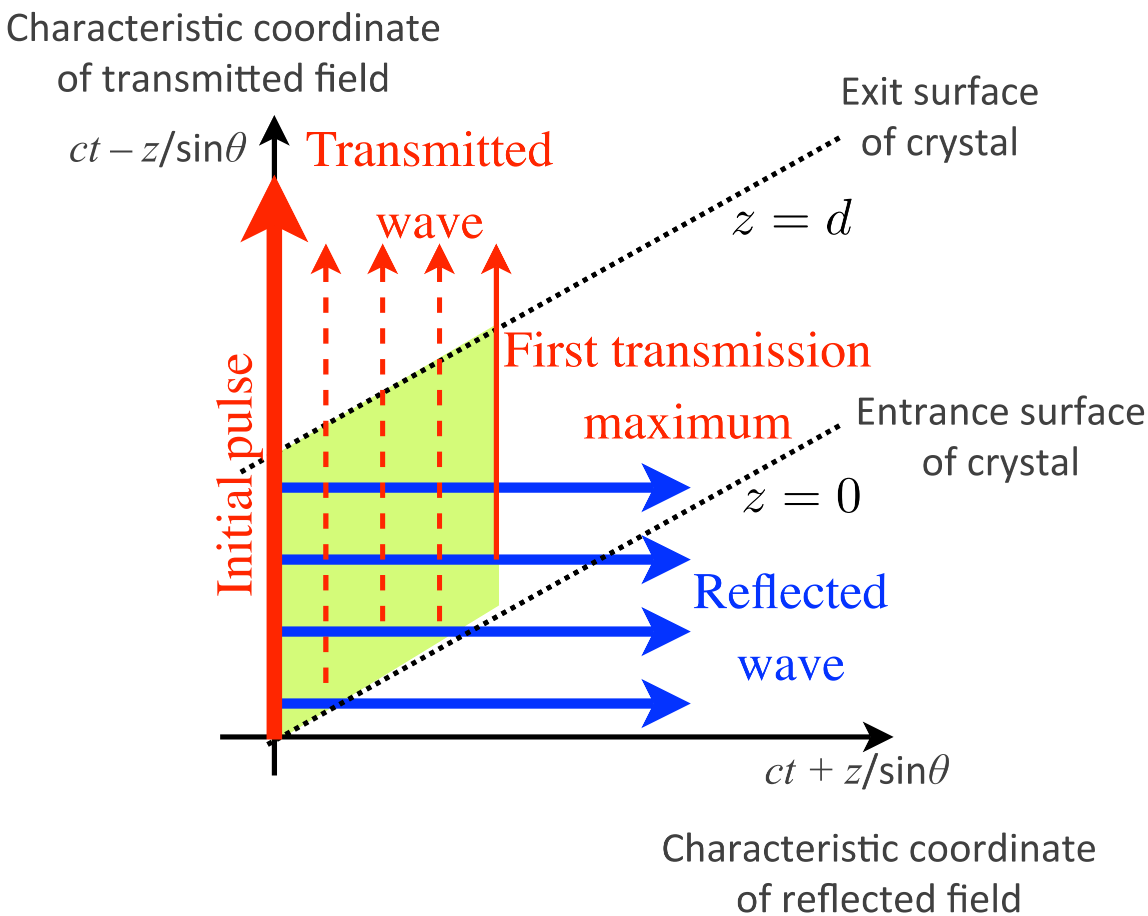
  Most are attributable to the "large" e-beam energy jitter ($\Delta\gamma/\gamma \sim 4 \times 10^{-4}$), but are there other sources?

- Nevertheless, seeding improves (ensemble averaged) spectral brightness within narrow seeded bandwidth
- Seeded mode available for user operations (J. Welch's talk today)
- First step towards a terawatt FEL

  Next step requires experimentally optimizing the predicted benefits of a post-saturation tapering of the undulator strength

Extra Slides

Time domain picture of self-seeding "wake"



Position of first peak proportional to **Interaction area**:
$\Delta t\, d/\sin\theta$ = constant

➔ time delay scales inversely with crystal thickness

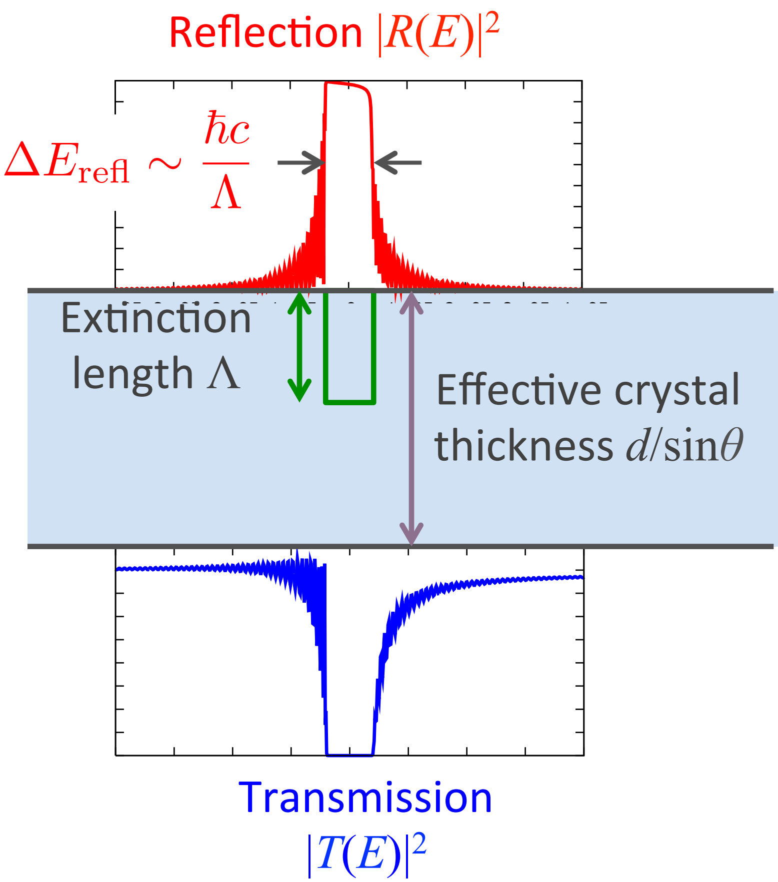
Seed amplitude scales with **Interaction length**

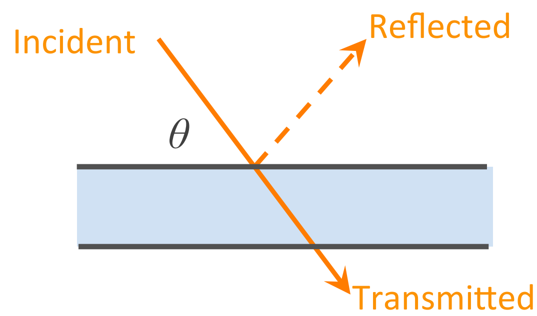
➔ Peak power scales quadratically with crystal thickness

† R.R. Lindberg and Yu. Shvyd'ko, *Phys. Rev. ST-Accel. Beams* **15**, 050706 (2012)

Bragg crystals in transmission for "wake" self-seeding

Bragg's law defines central energy of reflection $\lambda = \lambda_B \sin\theta$



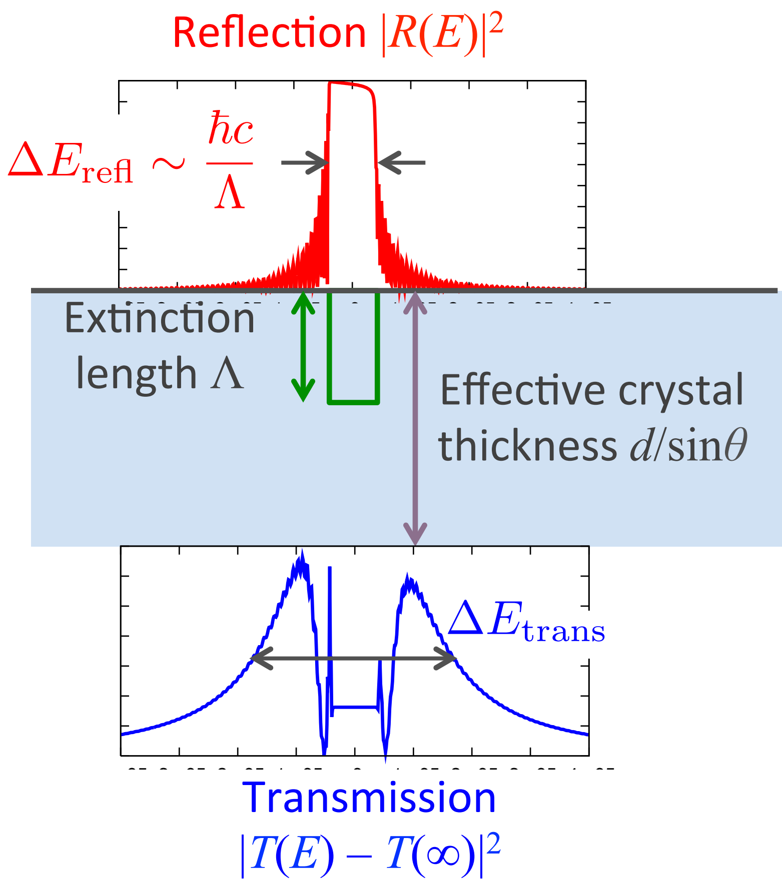


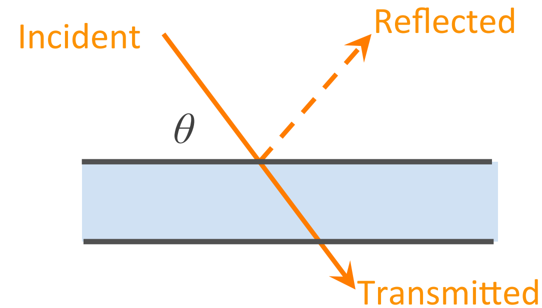
- Radiation has $\hbar/T_{\text{rad}} \gg \Delta E_{\text{refl}}$
  - ➔ Large Region of T contributes
- Seeding "wake" is determined by the difference $T(\mathrm{E}) - T(\infty)$

R.R. Lindberg and Yu. Shvyd'ko, *Phys. Rev. ST-Accel. Beams* **15**, 050706 (2012)

Bragg crystals in transmission for "wake" self-seeding

Bragg's law defines central energy of reflection $\lambda = \lambda_B \sin\theta$





- Radiation has $\hbar/T_{\text{rad}} \gg \Delta E_{\text{refl}}$
  - ➔ Large Region of T contributes
- Seeding "wake" is determined by the difference $T(\mathrm{E}) - T(\infty)$
- Relevant spectral components interact over entire crystal thickness

$$\Delta E_{\text{trans}} \sim \frac{d}{\Lambda \sin\theta} \Delta E_{\text{refl}}$$

$$\Delta t_{\text{trans}} \sim \frac{\Lambda^2 \sin\theta}{cd}$$

R.R. Lindberg and Yu. Shvyd'ko, *Phys. Rev. ST-Accel. Beams* **15**, 050706 (2012)