Population Inversion X-ray Laser Oscillator at LCLS and LCLS-II

Alex Halavanau, on behalf of XLO collaboration

FLS 2023 conference

XLO collaboration

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We are looking for collaborators in x-ray optics, please contact me (aliaksei@slac.stanford.edu)!

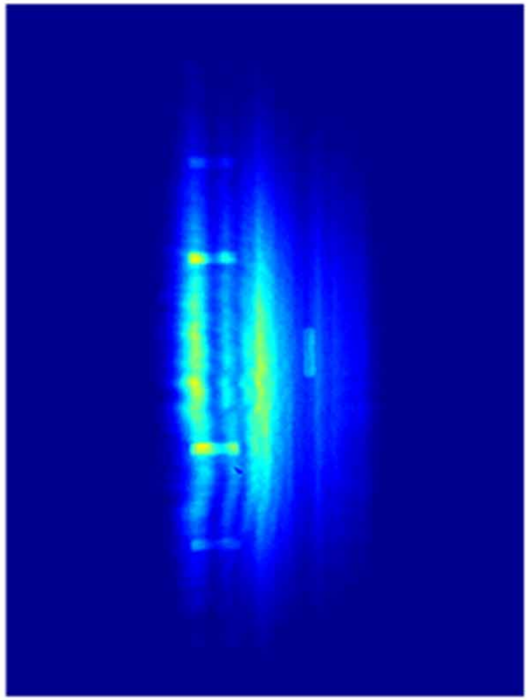
***principle investigators** **scientific advisors** theory/modeling gain medium delivery x-ray optics e-beam control analysis

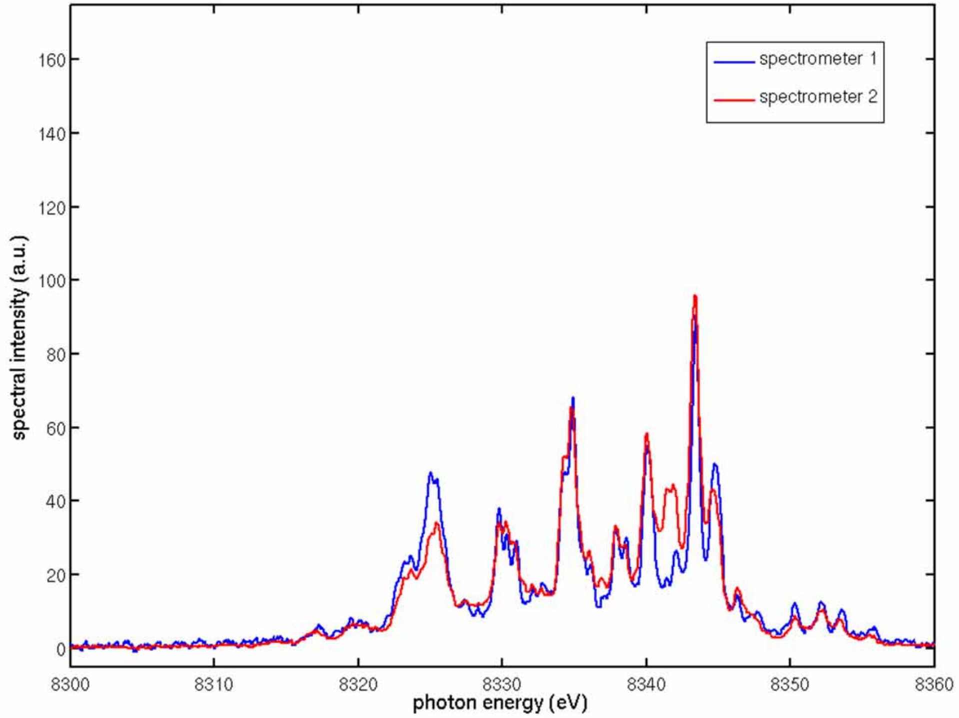
Project is funded by U.S. Department of Energy, BES office

This research uses resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC award ERCAP0020725.

Problem statement

How to improve hard x-ray coherence in XFELs?



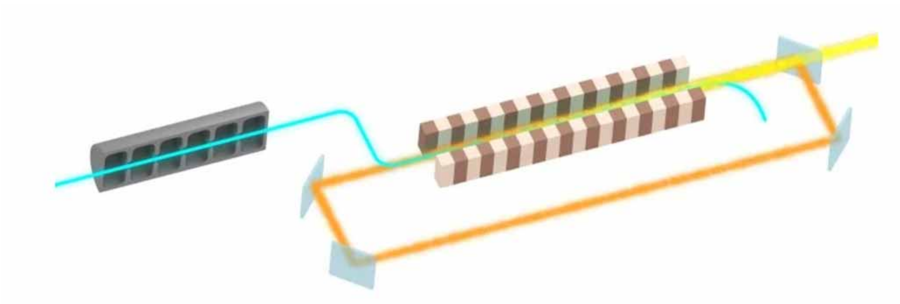


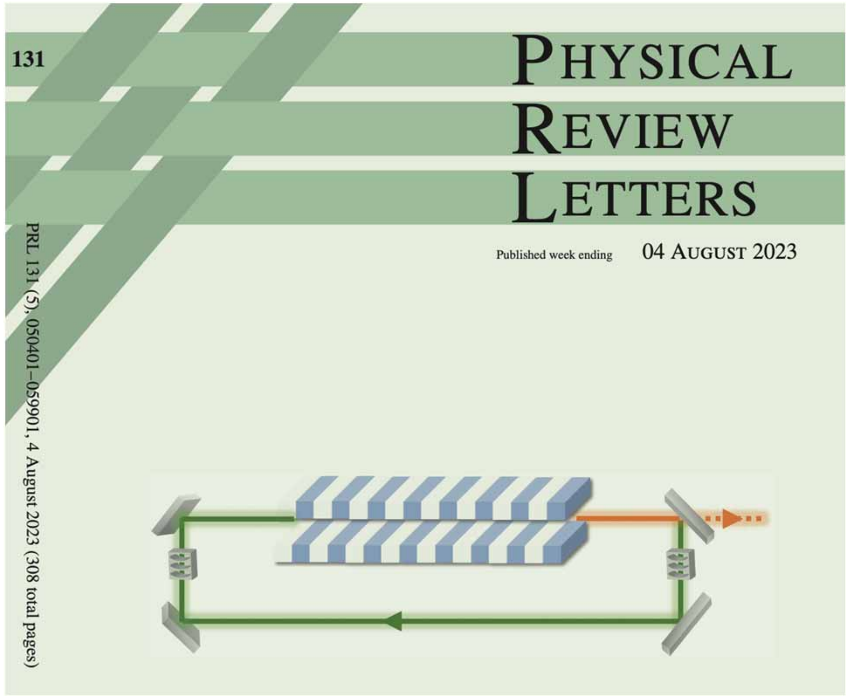
Typical SASE spectra at LCLS-HXR

LCLS-HXR pulse characteristics:

- Multi-spike (-mode) pulses
- High intensity (several mJ)
- 10-50 fs long, often chirped
- 10-20 eV wide
- Temporally incoherent
- Wavelength jitter

Cavity-based x-ray free-electron laser



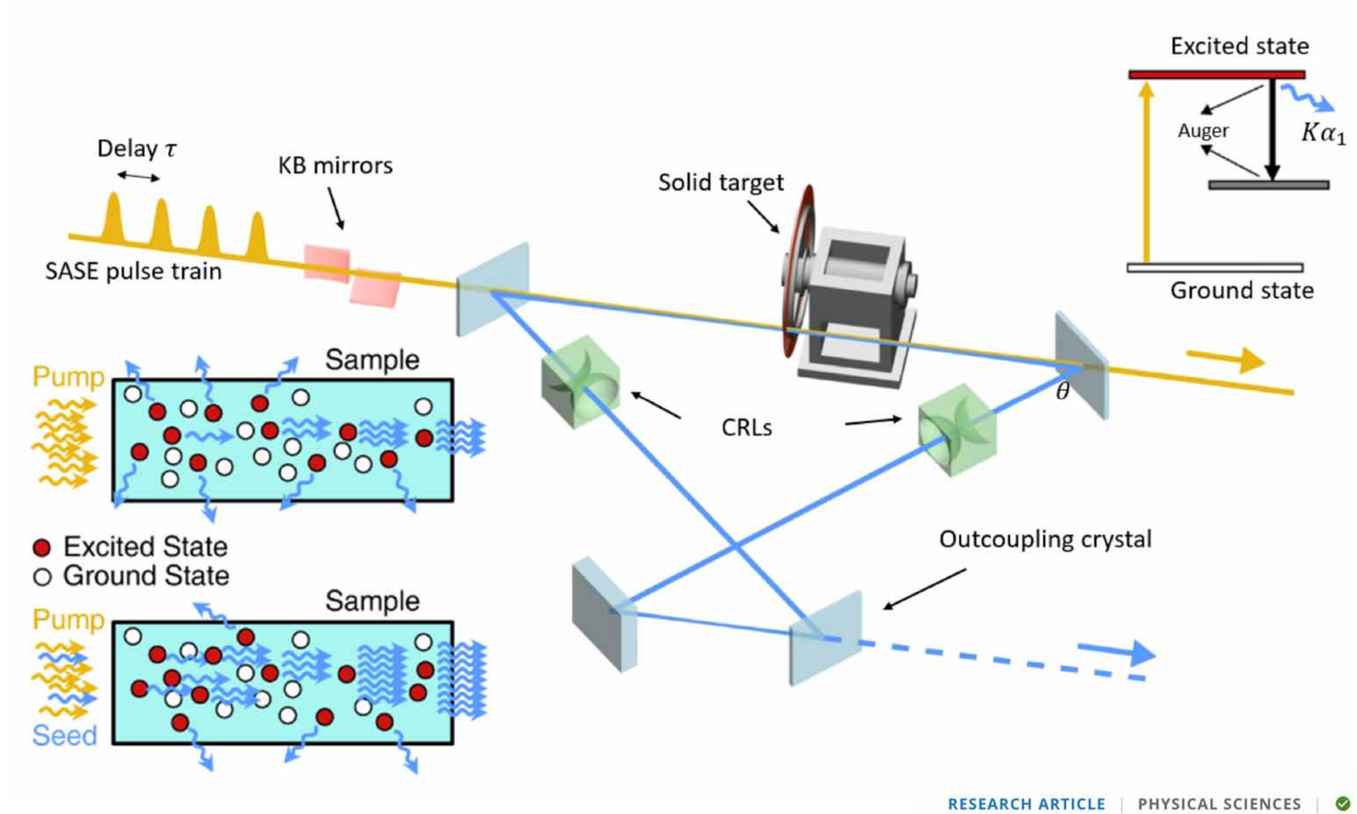


- Natural extension of XFELs analogous to classical lasers
- Two distinctive cases (low gain: XFELO, high gain: XRAFEL)
- Narrow-bandwidth, high-brightness pulses
- Temporally very coherent, better than self-seeding
- Low wavelength jitter

- Hard to build (never been done before for x-rays)
- Challenges in optics, outcoupling, e-beam quality
- Although tunable in theory, not really (very hard to do) tunable in practice

See talks by Zhirong Huang, Rachel Margraf, Jingyi Tang

XLO concept (2020) – population inversion x-ray laser



- Based on inner-shell population inversion (can be accomplished with an XFEL pump, yes, still need an XFEL)
- Low intensity (several uJ)
- 10-50 fs long, transform limited
- No wavelength jitter due to laws of QM
- PoP: 8 keV Cu K alpha1

Previous work on population inversion X-ray amplifiers by Yoneda (SACLA), Rohringer (LCLS), Bergmann (LCLS), Kroll (LCLS) paved the way for this research program

RESEARCH ARTICLE | PHYSICAL SCIENCES |

Population inversion X-ray laser oscillator

Aliaksei Halavanau, Andrei Benediktovitch, Alberto A. Lutman, +4, and Claudio Pellegrini Authors Info & Affiliations

Contributed by Claudio Pellegrini, May 13, 2020 (sent for review March 23, 2020; reviewed by Roger Falcone and Szymon Suckewer)

June 22, 2020 | 117 (27) 15511-15516 | https://doi.org/10.1073/pnas.2005360117

Modelling of XLO – general considerations

Approach in 1D FEL theory:

- Substitute electron distribution (*) into Vlasov equation (**)
- Calculate field evolution using SVEA Maxwell's equation (***)
- (Optional: recirculate in a cavity)

$$\psi(\eta,\theta,Z) = \frac{2\pi}{N_\lambda}\sum_{j=1}^{N_e}\delta(\eta-\eta_j)\delta(\theta-\theta_j) \qquad (*)$$

$$\frac{d\psi}{dZ} = \frac{\partial\psi}{\partial Z} + \frac{\partial\eta}{\partial Z}\frac{\partial\psi}{\partial\eta} + \frac{\partial\theta}{\partial Z}\frac{\partial\psi}{\partial\theta} = 0 \qquad (**)$$

$$\frac{\partial\psi}{\partial Z} + 2\eta\frac{\partial\psi}{\partial\theta} - D_2\left(Ae^{i\theta} + c.c.\right)\frac{\partial\psi}{\partial\eta} = 0$$

$$\frac{\partial A}{\partial Z} + \frac{\partial A}{\partial\theta} = D_1 e^{-i\theta}\int \psi(\eta,\theta,Z)d\eta \qquad (***)$$

Initial value challenge: charged particles sampling

Approach in 1D Maxwell-Bloch theory:

- Write down Maxwell's equation for polarized medium (SVEA) (*)
- Express polarization with dipole moment of 2 (n) level system (**)
- Evaluate dipole moment solving von-Neumann/Bloch equations (***)
- Recirculate in a cavity

$$\frac{\partial A(\theta,z)}{\partial z} = \frac{2\,\pi\,\omega\,i}{c}P(\theta,z) \qquad (*)$$

$$P(\theta,z) = 2\,n\sum_i \mu_i\rho^i(\theta,z)e^{\{\omega-\omega_i\}\theta} \qquad (**)$$

$$\dot{\boldsymbol{\rho}} = \frac{1}{i\hbar}[H,\boldsymbol{\rho}] \qquad (***)$$

Initial value challenge: correct fluorescence statistics

see talk by Kwang-Je Kim

Modelling of XLO – development of 3D code

Field evolution 3D Eqs.

$$\left[\frac{\partial}{\partial z} - \frac{i}{2k_0}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right) + \left(\frac{\mu(\mathbf{r},\tau)}{2} + i\delta(\mathbf{r},\tau)k_0\right)\right]\begin{pmatrix}\Omega^{(+)}_{s,\,\text{det.}}(\mathbf{r},\tau)\\ \Omega^{(+)}_{s,\,\text{noise}}(\mathbf{r},\tau)\end{pmatrix} = i\frac{3}{8\pi}\lambda^2\Gamma_{\text{rad.}}\begin{pmatrix} n(\mathbf{r})\sum_{e,g}T_{ges}\rho_{eg}(\mathbf{r},\tau)\\ f_s^{(+)}(\mathbf{r},\tau)\end{pmatrix},$$

$$\left[\frac{\partial}{\partial z} + \frac{i}{2k_0}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right) + \left(\frac{\mu(\mathbf{r},\tau)}{2} - i\delta(\mathbf{r},\tau)k_0\right)\right]\begin{pmatrix}\Omega^{(-)}_{s,\,\text{det.}}(\mathbf{r},\tau)\\ \Omega^{(-)}_{s,\,\text{noise}}(\mathbf{r},\tau)\end{pmatrix} = -i\frac{3}{8\pi}\lambda^2\Gamma_{\text{rad.}}\begin{pmatrix} n(\mathbf{r})\sum_{g,e}\rho_{ge}(\mathbf{r},\tau)T_{egs}\\ f_s^{(-)}(\mathbf{r},\tau)\end{pmatrix},$$

+ Bloch Eqs.

Stochastic modeling of x-ray superfluorescence

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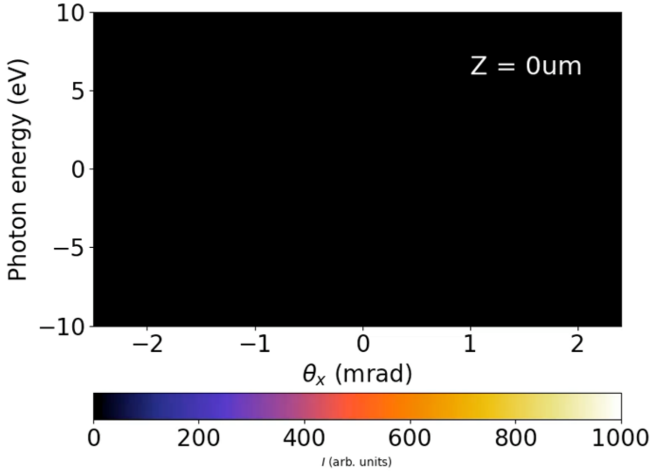
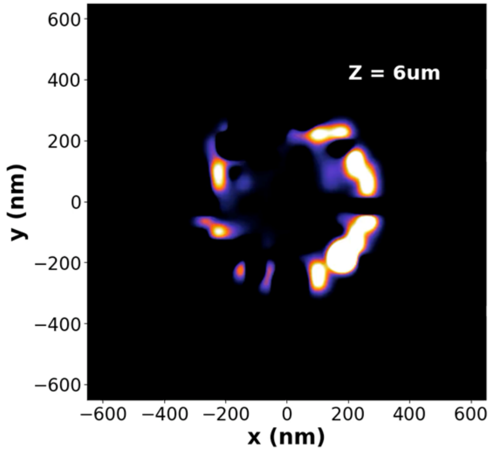
[4] *Department of Physics, Universität Hamburg, Hamburg 22761, Germany*

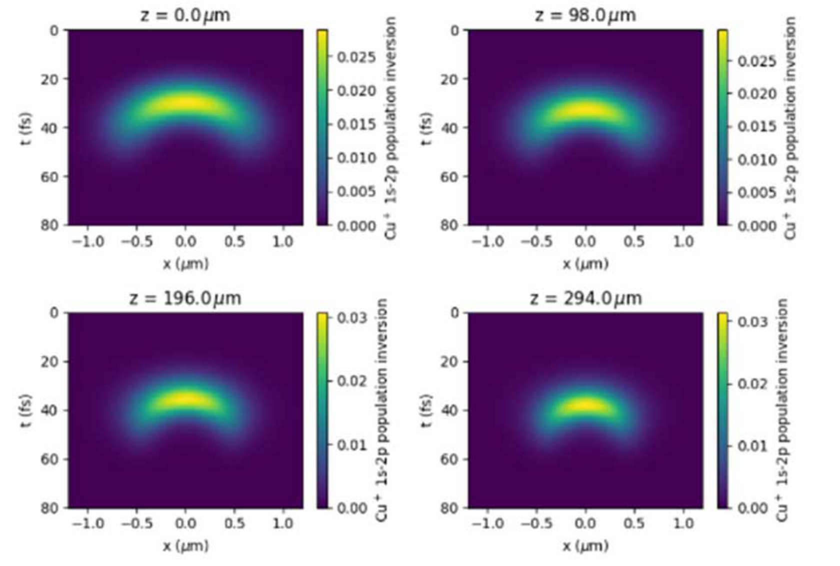
https://arxiv.org/abs/2303.00853



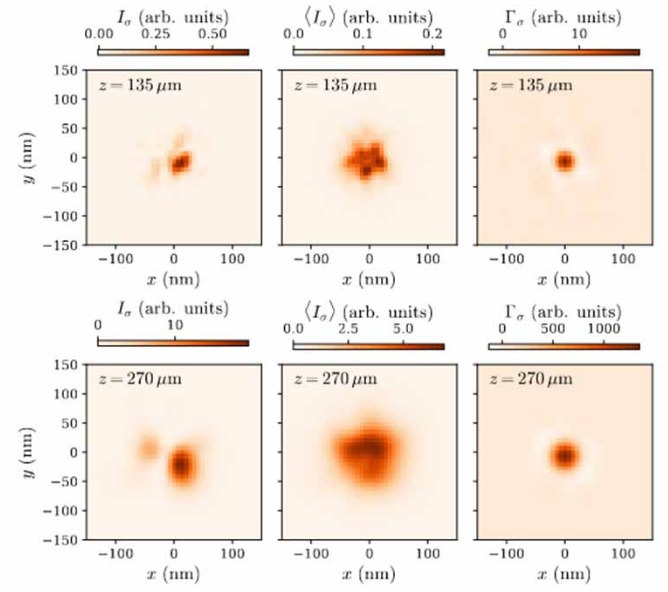


This effort is comparable to writing a 3D time-dependent FEL code from scratch

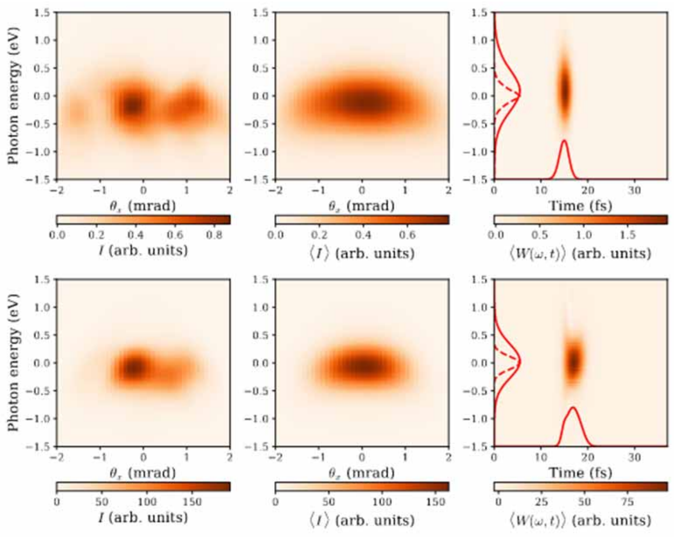
Modelling of XLO – single pass effects



Non-linear gain as a function of r (ideal sim.)



Spatial coherence as a function of target thickness

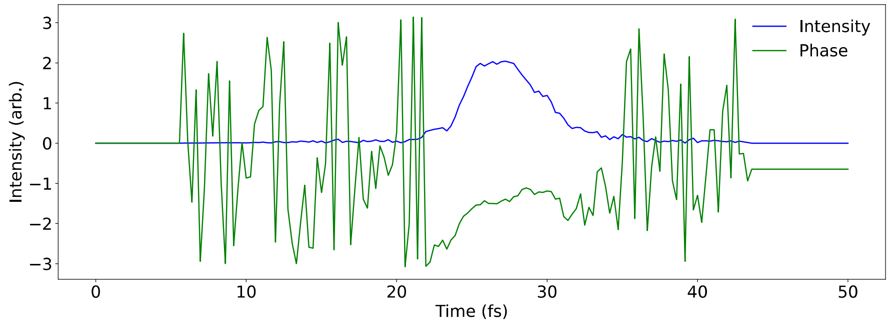


Spectral-angular-temporal properties

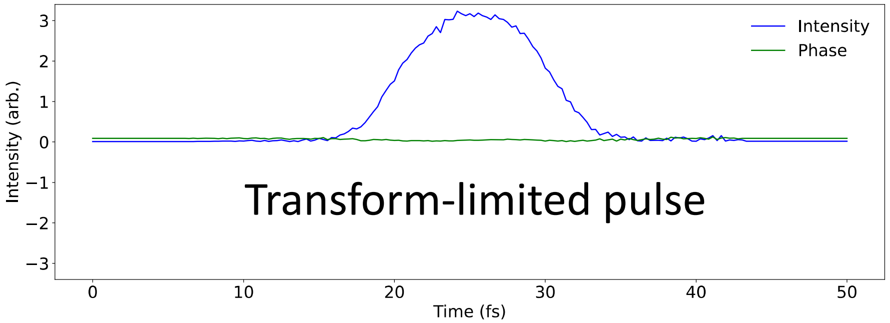
- Similar to FEL and other lasers, this process has 3D effects due to non-linearity of the gain

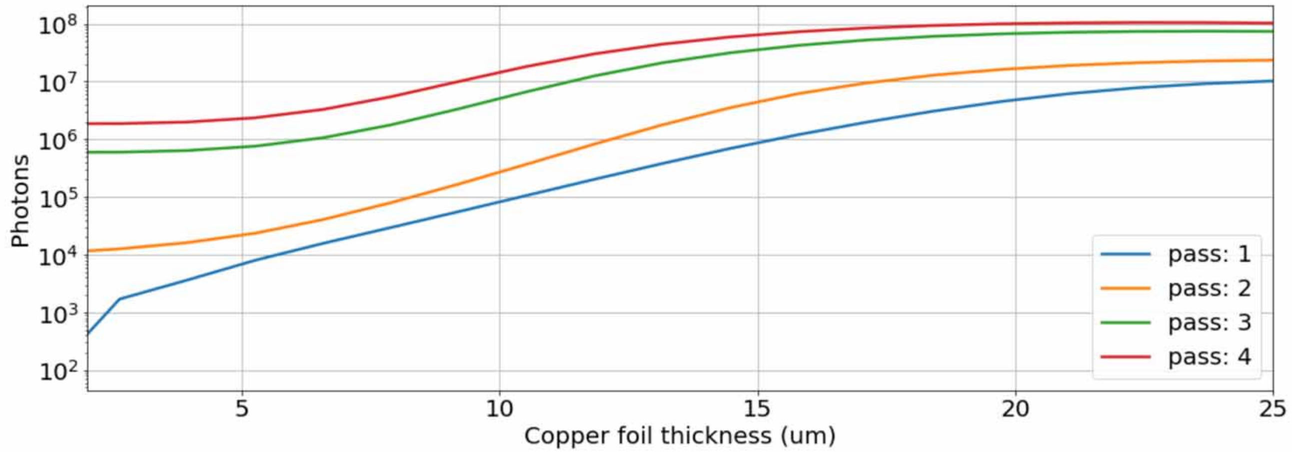
Modelling of XLO – cavity recirculation

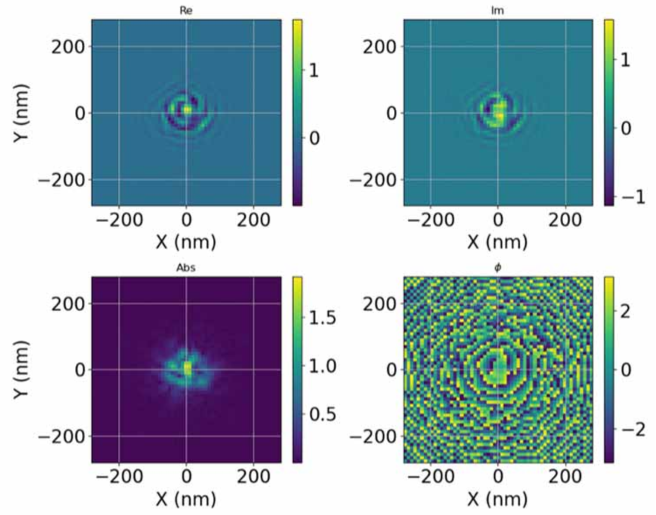
Pass 1



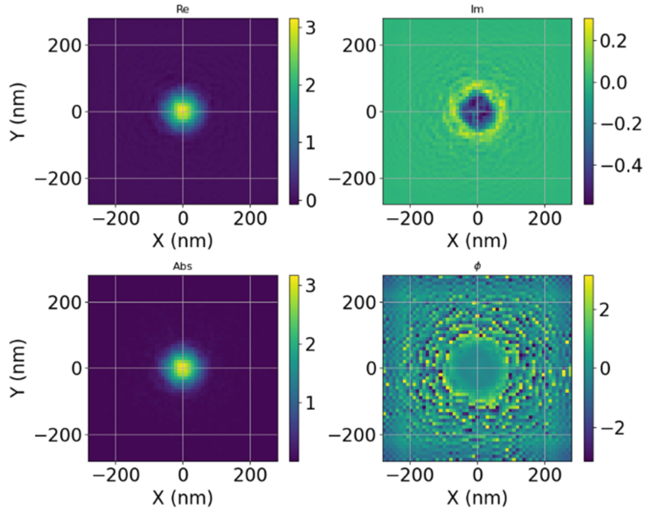
Pass 4







Pass 1



Pass 4

Field propagation in z

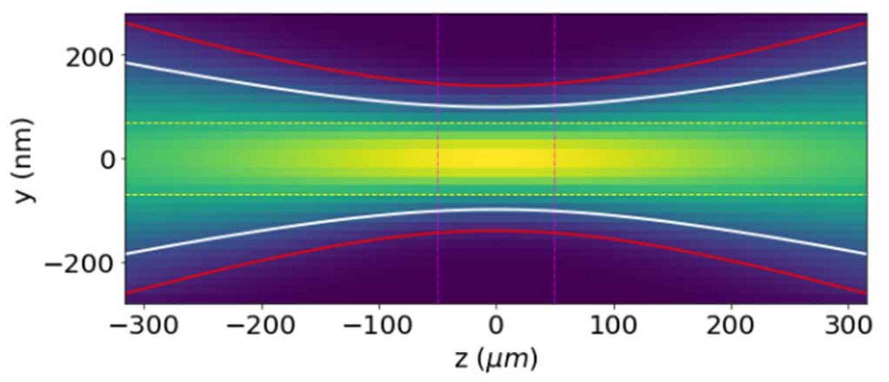
$$\frac{\partial}{\partial z}\mathcal{E} - \frac{\mathrm{i}}{2k}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\mathcal{E} = -\frac{\kappa}{2}\mathcal{E} + c\rho$$

→ $\mathcal{E}$, κ, ρ are functions of x,y,z,τ (in the following x,y,τ omitted for simplicity); k,c are const.

The equation can be rewritten as

$$\frac{\partial}{\partial z}\mathcal{E} = L\mathcal{E} + c\rho,$$

where $L = \frac{\mathrm{i}}{2k}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\kappa}{2}$



Using split-operator method from QM:

Final expression:

$$\mathcal{E}(z+\Delta z) = e^{-\frac{\Delta z}{4}\kappa(z+\Delta z)} FT^{-1}\left[e^{-\frac{i\Delta z}{2k}\left(k_x^2+k_y^2\right)} FT\left[e^{-\frac{\Delta z}{4}\kappa(z)}\mathcal{E}(z)\right]\right] + c\rho(z+\Delta z)$$

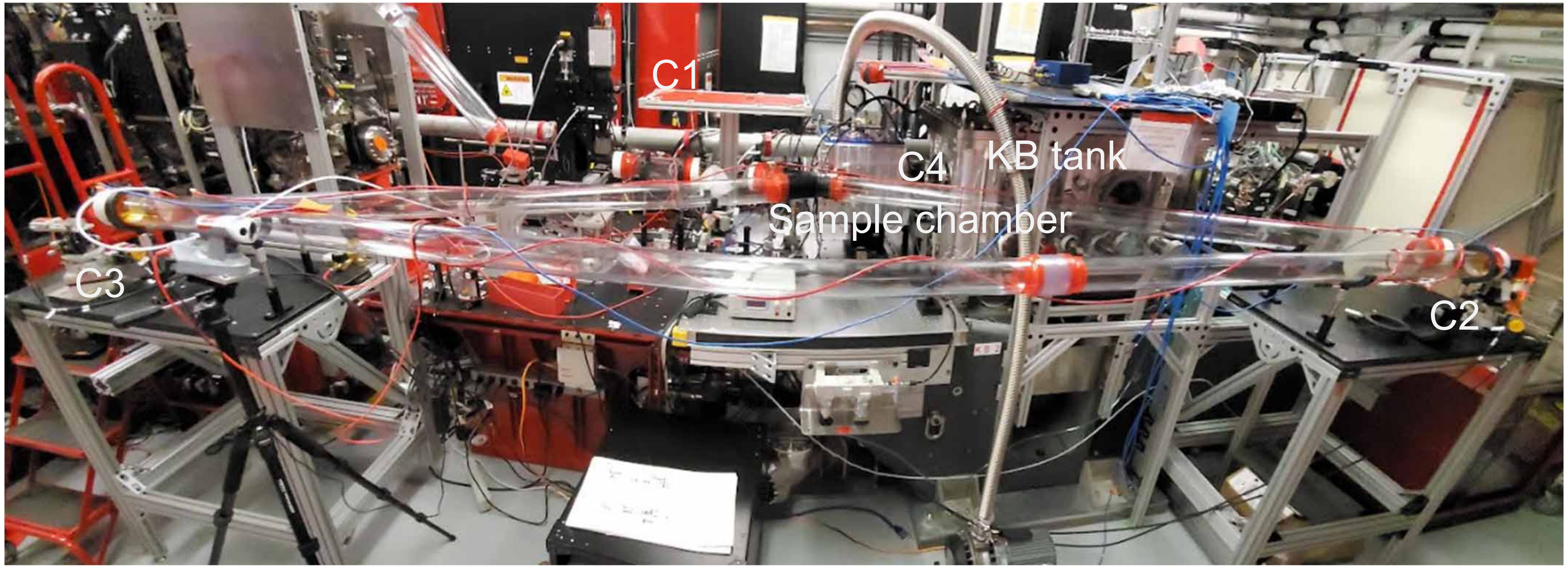
Need special treatment for propagating inside the cavity by removing the quadratic phase component

$$\varepsilon(z+dz) = \varepsilon'(z'+dz') * FW(z,z')$$

to be published soon

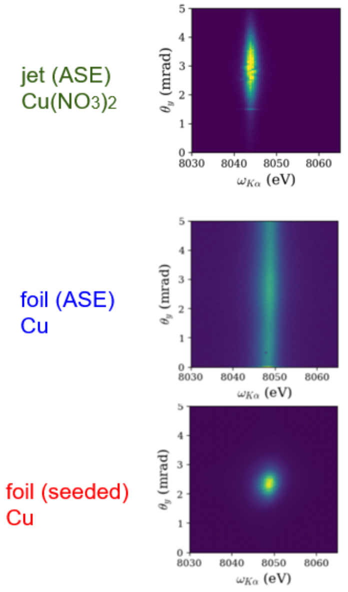
XLO cavity first prototype at LCLS-CXI end-station

Time of flight is 35 ns



October, 2022

First experimental results



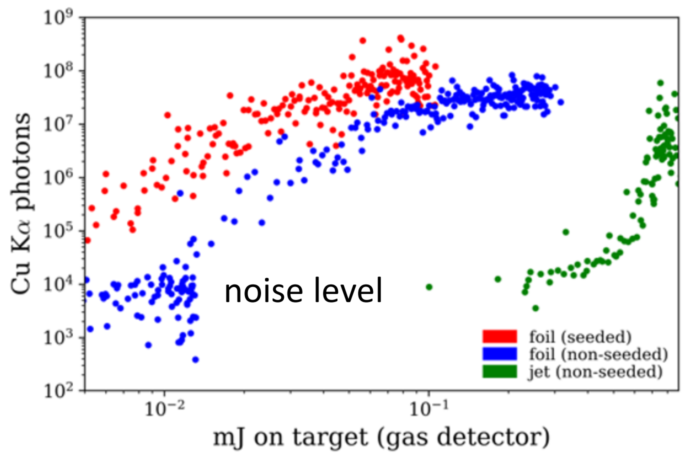
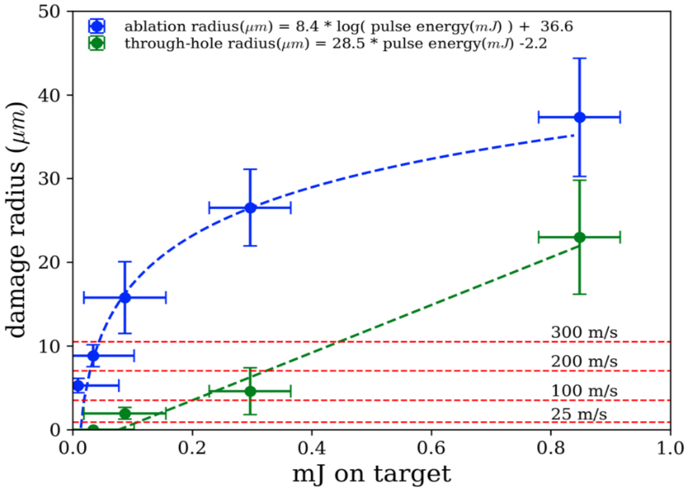
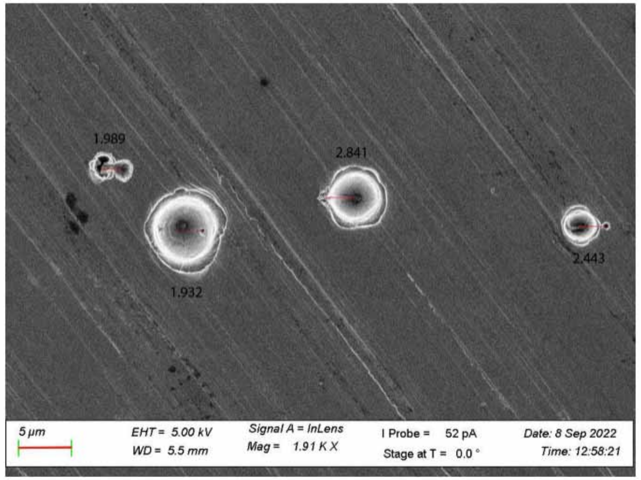


Table 1: Measured and calculated XLO cavity crystals transmission at 8.048 keV. *- limited by the detector aperture.

Beam transport	Measured, %	Theoretical, %
After flat C1	0.65	0.7
Flat C1 - C2	62	65
Curved C1 – C2	27	To be verified
Flat C1-C2-C3	*	0.6
Curved C1-C2-C3	2.2	To be verified
After C4	To be verified	56
Total	To be verified	≈ 0.01

Gain medium damage



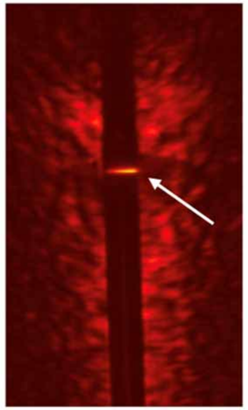


LCLS two-pulse mode (35 ns)

Development of XLO gain medium

Paper accepted in Review of Scientific Instruments

Liquid jets – not a very good option (v1)

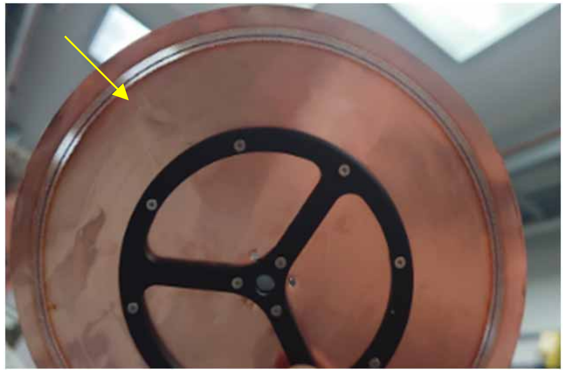


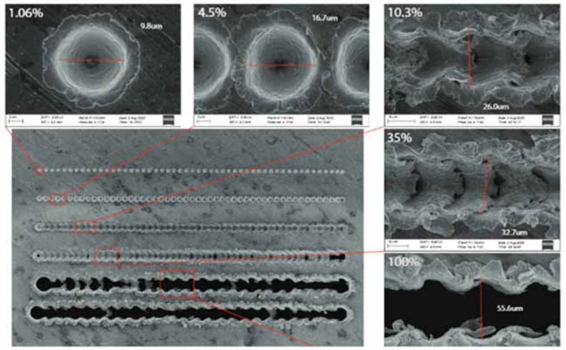
XFEL excited volume

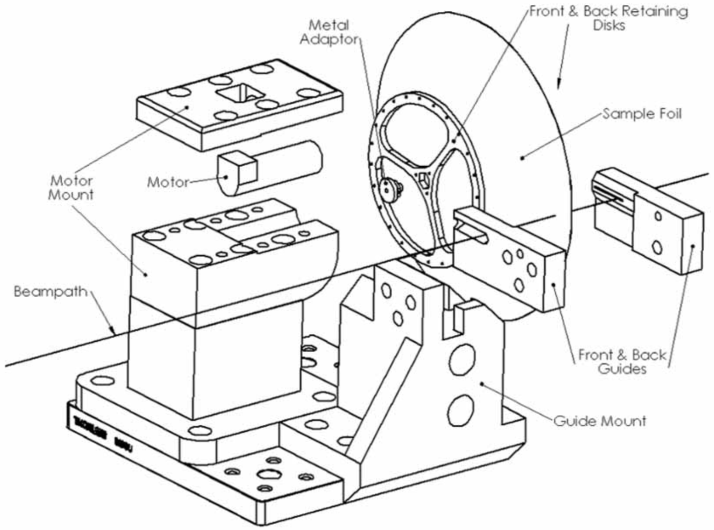
Jet image in 640 nm transmission light

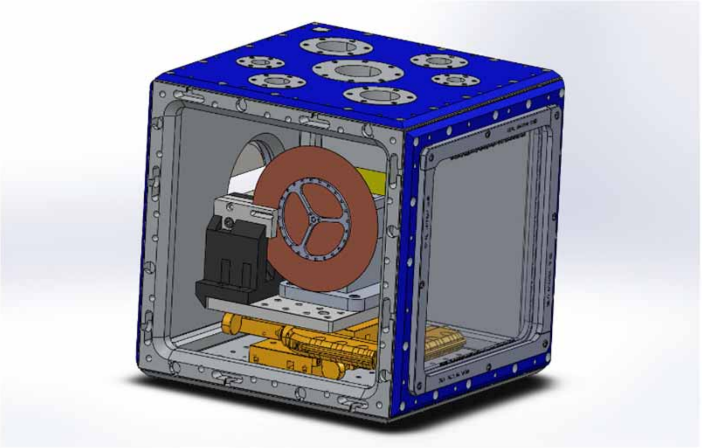
It is hard to move 200 um jet with 300 m/s

Solid copper disk – a better option (v1.2)



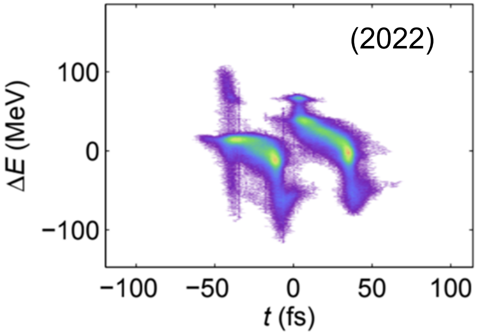


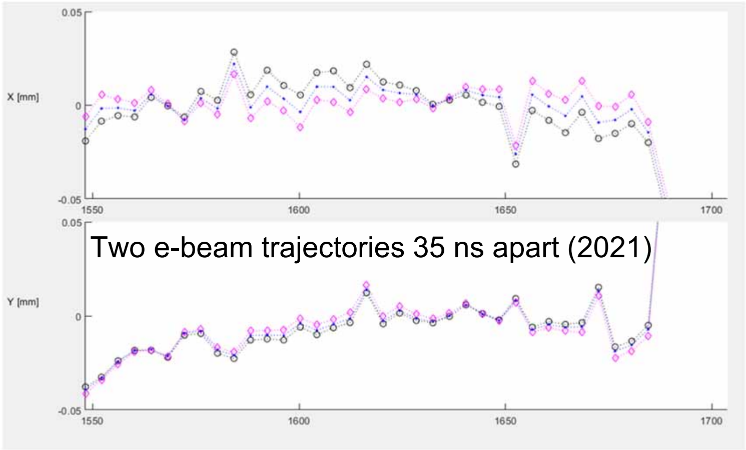


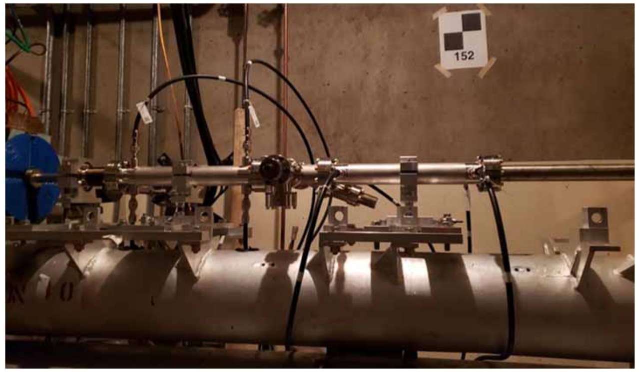


LCLS multi-bunch improvement

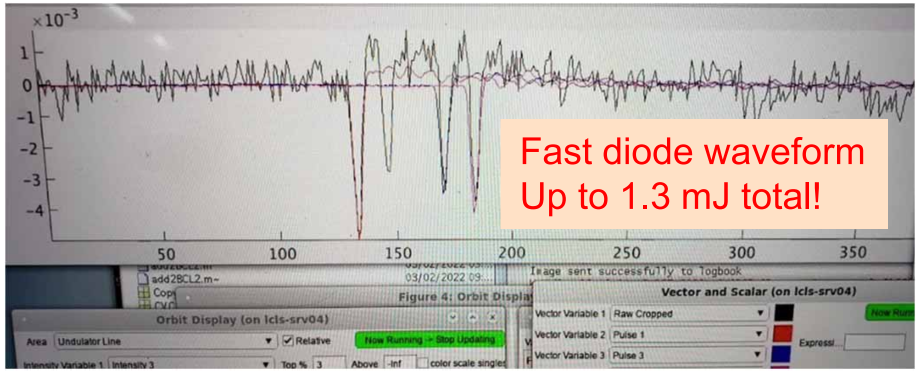
- Initial RAFEL gain demonstration will be done with 2 pulses, 35 ns apart
- XLO in saturation will require 4 and possibly more pulses. A Multi-pulse R&D program is currently underway at SLAC
- Multi-bunch control with TEM striplines

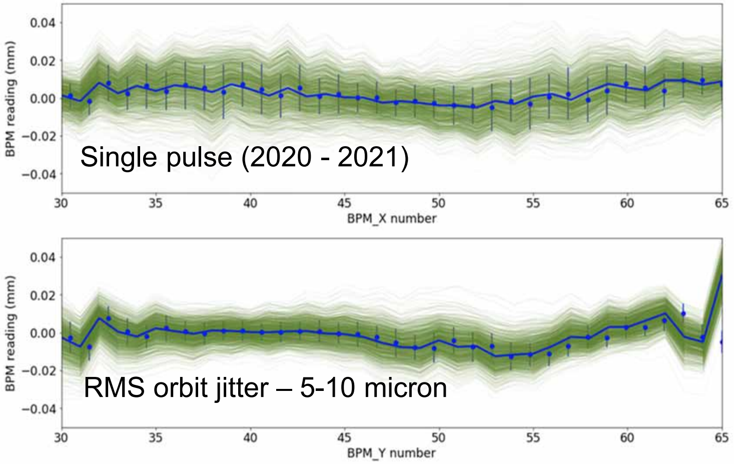






TEM striplines installed during winter 2021/2022

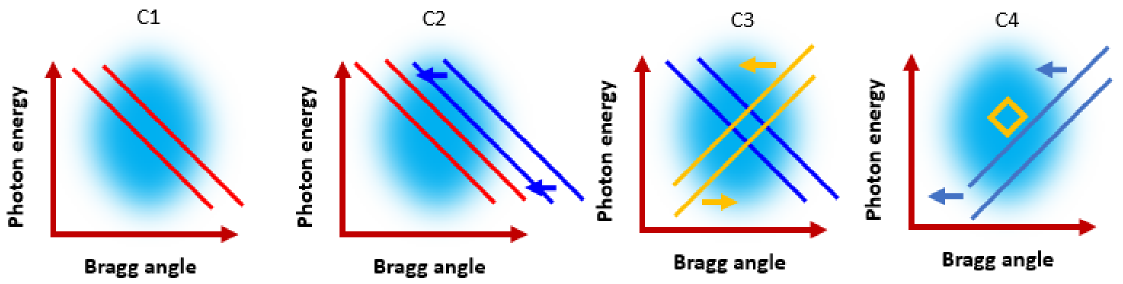




Decker, F.-J. *et al*, **Tunable x-ray free electron laser multi-pulses with nanosecond separation**
Scientific Reports, **12**, 3253 (2022)

XLO cavity alignment

Alignment process can be characterized in this diagram



Broad rocking curve, large signal

Narrow rocking curve, large signal

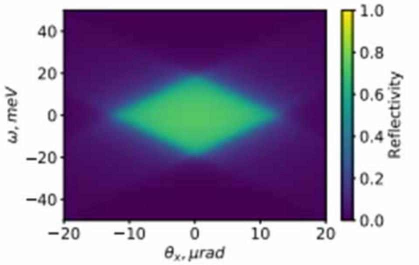
Broad rocking curve, small signal

Narrow rocking curve, small signal

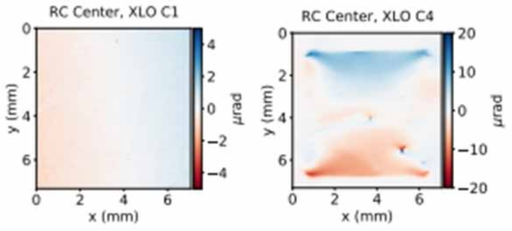
$$R(\Delta\theta,\theta,\omega) = \eta - sgn\left[\mathrm{Re}(\eta)\right]\sqrt{\eta^2-1}\sqrt{\frac{|F_H|}{|F_{\bar{H}}|}},$$

and η is given by:

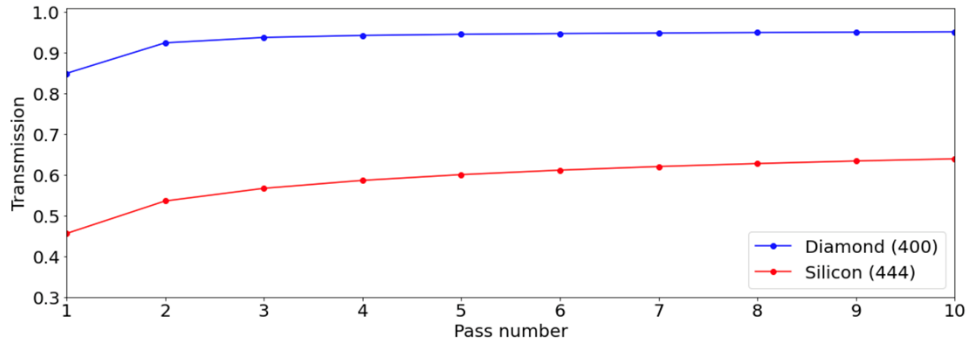
$$\eta(\Delta\theta,\theta,\omega) = \frac{(-\Delta\theta + \tan\theta\ \ \Delta\omega/\omega_0)\sin 2\theta - \Gamma F_0}{\Gamma|P|\sqrt{F_H F_{\bar{H}}}}$$



Need high quality crystals ->



Cavity efficiency (after initial 0-th roundtrip)



Article | Published: 14 August 2023

Low-loss stable storage of 1.2 Å X-ray pulses in a 14 m Bragg cavity

Rachel Margraf, River Robles, Alex Halavanau, Jacek Kryzywinski, Kenan Li, James MacArthur, Taito Osaka, Anne Sakdinawat, Takahiro Sato, Yanwen Sun, Kenji Tamasaku, Zhirong Huang, Gabriel Marcus & Diling Zhu

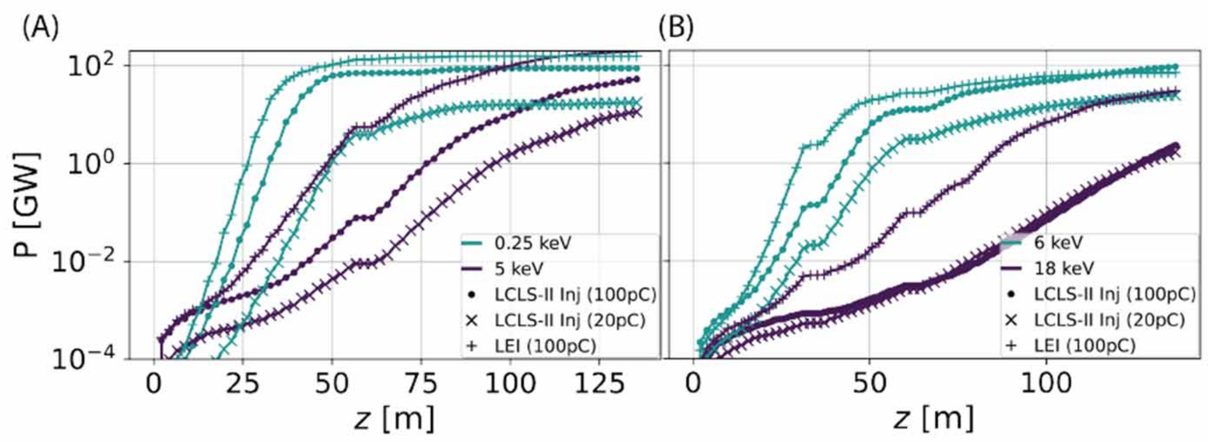
Alignment of a rectangular cavity at 10 keV is presented here

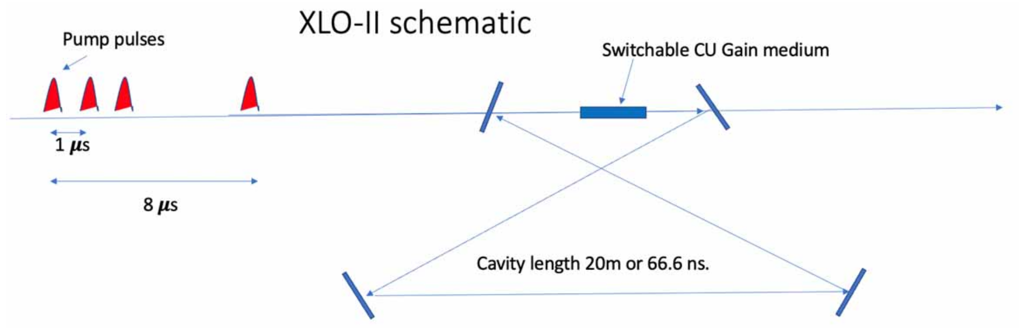
XLO-II (operation with LCLS-II-HE)

- Since we operate in high gain regime, we can recirculate the radiation in the cavity a number of times

- In this case, the limitations are:

➢ losses in the cavity per turn (need to consider diamond crystals instead of Silicon)
➢ Pulse intensity of LCLS-II-HE
➢ Average heat load on optics (<200 W)





Diamond	Bragg angle, θ_B(deg)	$\Delta\theta$ (μrad)	$\Delta\omega$ (meV)	$\Delta\omega/\omega \times 10^{-6}$	τ (fs)
311	45.7	9.6	75.4	9.4	23.9
400	59.8	14	65.6	8.1	27.4
331	70.3	13	37.4	4.7	48.1

Conclusions and outlook

- XLO is a vibrant collaboration aimed to build and commission the first population inversion x-ray laser oscillator (funded by BES-DOE)
- In our first experiments we made significant progress. The initial results show no roadblocks, but more work is still to be done
- The main challenges for building XLO are the gain medium damage and the intra-cavity focusing, outcoupling, alignment
- XLO will be an important addition to the existing or planned coherent X-ray sources, with interesting pulse properties. We are looking now at its applications for advanced x-ray imaging and fundamental optics studies.
- Operation of XLO using LCLS-II-HE/X operation will provide a high repetition rate, up to 10 kHz, fully coherent, X-ray laser oscillator
- Design of first experiments is underway