

X-ray FEL oscillator

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Outline

- Introduction to the x-ray free-electron laser oscillator (XFELO)
- Linear physics of an XFELO
 - 3D gain from Madey's-type formula
 - Longitudinal supermodes
- Optimization of the driving electron beam for XFELO at the LCLS
- Development of enabling technologies for an XFELO
- Role of fluctuations and imperfections on steady-state operation
- Ultimate limits to XFELO stability
- Possibility for a frequency stabilized, mode-locked x-ray laser

Level of understanding Most sophisticated

X-ray FEL oscillator is comparable to optical laser



⁺ R. Colella and A. Luccio, *Opt. Comm.* **50**, 41 (1984)
K.-J. Kim, Y. Shvyd'ko, and S. Reiche, *Phys. Rev. Lett.* **100**, 244802 (2008)

XFELO is complementary to high-gain FELs based on self-amplified spontaneous emission (SASE)

Characteristic	SASE	XFELO
Pulse duration	1 to 200 fs	200 to 2000 fs
Photons/puse	~10 ¹²	~10 ⁹
Energy BW	~ 10 eV	~10 ⁻² eV
Coherence	Transverse	Fully
Repetition rate	Variable	~ MHz
Stability	1-100% depending on chosen BW	< 1%
Brightness	~10 ³²	~10 ³²

XFELO Science

- 1. Inelastic x-ray scattering
- 2. Nuclear resonant scattering
- 3. X-ray photoemission spectroscopy
- 4. Hard x-ray imaging
- 5. X-ray photon correlation spectroscopy

XFELO will revolutionize techniques pioneered at 3rd generation light sources, complement the capabilities of SASE FELs, and may enable optical techniques to be applied at x-ray wavelengths

Single-pass FEL gain in 3D:

Continuity equation for the electron distribution function



Take Fourier transform w.r.t. longitudinal coordinate θ and linearize:

 $F \to \overline{F}(\boldsymbol{x}, \gamma, \boldsymbol{p}; z) + F_{\omega}(\boldsymbol{x}, \gamma, \boldsymbol{p}; z)$

Smooth, time-independent background distribution

Component of distribution at frequency ω (bunching)

 $\left[\frac{\partial}{\partial z} + i\left(2k_uh\frac{\Delta\gamma}{\gamma} - \frac{k_h}{2}\boldsymbol{p}^2\right) + \boldsymbol{p}\cdot\frac{\partial}{\partial\boldsymbol{x}}\right|F_{\omega} = -\chi_h E_{\omega}\frac{\partial}{\partial\gamma}\bar{F}$

Single-pass FEL gain in 3D: Solution for F by integrating over the characteristics

$$\begin{bmatrix} \frac{\partial}{\partial z} + i\left(2k_{u}h\frac{\Delta\gamma}{\gamma} - \frac{k_{h}}{2}p^{2}\right) + p \cdot \frac{\partial}{\partial x} \end{bmatrix} F_{\omega} = -\chi_{h}E_{\omega}\frac{\partial}{\partial\gamma}\bar{F}$$

$$e^{-i(2k_{u}h\Delta\gamma/\gamma - k_{h}p^{2}/2)z} \frac{d}{dz}\Big|_{\boldsymbol{x}=\boldsymbol{x}_{0}+\boldsymbol{p}_{0}z} e^{i(2k_{u}h\Delta\gamma/\gamma - k_{h}p^{2}/2)z}F_{\omega} \quad \text{and integrate...}$$

$$F_{\omega}(z) = e^{-i(2k_{u}h\Delta\gamma/\gamma - k_{h}p^{2}/2)z}F_{\omega}(0)$$

$$-\chi_{h}\int_{0}^{z} ds \ e^{-i(2k_{u}h\Delta\gamma/\gamma - k_{h}p^{2}/2)(z-s)}E_{\omega}(\boldsymbol{x}-\boldsymbol{p}s,\boldsymbol{p};s)\frac{\partial}{\partial\gamma}\bar{F}(\boldsymbol{x}-\boldsymbol{p}s,\boldsymbol{p},\gamma;s)$$

Single-pass FEL gain in 3D: Paraxial equation for radiation (in angular rep.)

$$\left[\frac{\partial}{\partial z} + ik_u \frac{\Delta \omega}{\omega_1} + \frac{ik}{2} \boldsymbol{\phi}^2\right] \mathcal{E}_{\omega}(\boldsymbol{\phi}, z) = -\kappa_h n_e \int d\gamma d\boldsymbol{p} d\boldsymbol{x} \ F_{\omega}(\gamma, \boldsymbol{x}, \boldsymbol{p}; z) e^{-ik\boldsymbol{x}\cdot\boldsymbol{\phi}}$$

Integrate over undulator length:



Solution for the radiation field

Input field

$$\mathcal{E}_{\omega}(\phi, L_{u}) = \underbrace{e^{-i(k_{u}\Delta\omega/\omega_{1}+k\phi^{2}/2)L_{u}}\mathcal{E}_{\omega}(\phi, 0)}$$
 Spontaneous radiation

$$- \kappa_{h}n_{e} \int_{0}^{L_{u}} dz \ e^{-i(k_{u}\Delta\omega/\omega_{1}+k\phi^{2}/2)(L_{u}-z)} \int d\gamma d\mathbf{p} d\mathbf{x} \ e^{-ik\mathbf{x}\cdot\phi} e^{-i(2k_{u}h\Delta\gamma/\gamma-k_{h}\mathbf{p}^{2}/2)z} F_{\omega}(0)$$

$$+ \kappa_{h}\chi_{h}n_{e} \int_{0}^{L_{u}} dz \ e^{-i(k_{u}\Delta\omega/\omega_{1}+k\phi^{2}/2)(L_{u}-z)} \int d\gamma d\mathbf{p} d\mathbf{x} \ e^{-ik\mathbf{x}\cdot\phi}$$

$$\times \int_{0}^{z} ds \ e^{-i(2k_{u}h\Delta\gamma/\gamma-k_{h}\mathbf{p}^{2}/2)(z-s)} E_{\omega}(\mathbf{x}-\mathbf{p}s,\mathbf{p};s) \frac{\partial \bar{F}}{\partial \gamma}$$
FEL gain!
When the gain is small, we can get a closed form solutionby replacing E_{ω} here with its initial value

Single-pass FEL gain in 3D:

3D Madey's theorem for the harmonic gain (G is small)

Gain is a convolution over the input radiation, undulator field, and electron beam distribution/brightness functions[†]

$$G = \frac{n_e \chi_h \kappa_h}{\lambda^2} \frac{\int d\eta d\mathbf{p} d\boldsymbol{\phi} d\mathbf{x} d\mathbf{y} \ \mathcal{B}_E(\mathbf{y}, \boldsymbol{\phi}) \mathcal{B}_U(\eta, \mathbf{x} - \mathbf{y}, \boldsymbol{\phi} - \mathbf{p}) \frac{\partial}{\partial \gamma} \bar{F}(\gamma, \mathbf{x}, \mathbf{p})}{\int d\boldsymbol{\phi} d\mathbf{y} \ \mathcal{B}_E(\mathbf{y}, \boldsymbol{\phi})}$$

(Wigner function)

Assume Gaussian field in position, angle

Single electron undulator brightness (Wigner function) Known

Electron beam distribution function

Assume Gaussian in position, angle, energy

When the dust settles...

$$G = \frac{I}{I_A} \frac{\pi h K^2 [\mathrm{JJ}]_h^2 L_u^3}{\gamma^3 \lambda_u \Sigma_x^2} \int_{-1/2}^{1/2} ds dz \ e^{-2[2\pi N_u(z-s)h\sigma_\gamma/\gamma]^2} \frac{(z-s)\left\{\sin[2x(z-s)] - i\cos[2x(z-s)]\right\}}{1 + zs\frac{L_u^2 \Sigma_\phi^2}{\Sigma_x^2} - i(z-s)\left[kL_u \Sigma_\phi^2 + \frac{L_u}{4k\Sigma_x^2}\right]}$$

⁺ K.-J. Kim, Nucl. Instrum. Methods Res. A **318**, 489 (1992)

Single-pass FEL gain in 3D:

Analytic formula for a Gaussian laser and electron beam



$$\Sigma_x^2 \equiv \sigma_x^2 + \sigma_r^2 \qquad \qquad \Sigma_\phi^2 \equiv \sigma_p^2 + \sigma_\phi^2$$

For a given set of e-beam and undulator parameters we can numerically maximize the gain G with respect to the

- 1. Electron focusing $Z_{\beta} = \sigma_x^2 / \epsilon_x$ (β-function at undulator middle)
- 2. Radiation Rayleigh length $Z_R = \sigma_r^2 / (\lambda / 4\pi)$
- 3. Frequency difference from resonance $x = \pi N_u \Delta \omega / \omega$

Single-pass FEL gain in 3D

Gain is maximized when the electron and $G/G_{\rm max}$ 0.5 laser beams have maximal overlap 1.0E-beam envelope 0.4 0.9 Z_R/L_u Laser envelope 0.3 0.8 0.2 0.7 And when the beam nearly matches the 0.1 spontaneous radiation "mode" size 0.2 0.3 0.40.5 0.1 $Z_{\beta} = Z_R \sim \frac{L_u}{}$ Z_{β}/L_{u} Electron beam requirements High brightness: $\varepsilon_r \le 0.3 \ \mu m$, $\Delta \gamma / \gamma \le \text{few} \times 10^{-4}$ Relatively low intensity: $I_{\text{peak}} \sim 10 - 200 \text{ A}$ Single pass gain ~ 0.3 to 2 Moderate duration: 0.2 – 5 ps Repetition rate = $c/(cavity length) \sim MHz$ Undulator parameters: $K \sim 1$ and $N_{\mu} \sim 10^3$

Longitudinal dynamics of an XFELO: Model of the Bragg crystal reflectivity



Bragg crystals work via coherent scattering of photons whose wavelength approximately satisfies Bragg's Law, $\lambda = 2d \cos\theta$ Many crystal planes contribute, $N_p \sim 10^5 - 10^8$, and the region of high reflectivity has a bandwidth $\Delta\lambda/\lambda \sim N_p^{-1} < 10^{-5}$



Longitudinal dynamics of an XFELO: Linear supermodes[†] of the exponential gain regime

Gain approximately follows electron beam current: $G(t) \approx Ge^{-t^2/2\sigma_e^2} \approx G(1 - t^2/2\sigma_e^2)$

The change of the radiation field E(t,n) on pass *n* is approximately described by

$$\frac{\partial}{\partial n}E(t,n) = E(t,n) + \underbrace{\frac{G}{2}\left(1 - \frac{t^2}{2\sigma_e^2}\right)}_{e}E(t,n) - \underbrace{\left(\frac{R}{2} - \frac{1}{\sigma_\omega^2}\frac{\partial^2}{\partial t^2}\right)}_{e}E(t,n) + \underbrace{\ell\frac{\partial}{\partial t}}_{e}E(t,n)$$

Gain due to finite electron beam

Loss and filtering due to Bragg crystal

Delay

General solution is spanned by a sum of Gauss-Hermite modes

$$E_m(t,n) = e^{\Lambda_m n} e^{-t^2 \sigma_\omega^2 \ell/2} \exp\left(-\frac{\sqrt{G}\sigma_\omega}{2\sigma_e} t^2\right) H_m\left(G^{1/4}\sqrt{\frac{\sigma_\omega}{\sigma_e}} t\right)$$

Effective single pass gain with $\Lambda_m \equiv \frac{1}{2} \left[1 + G - R - \frac{\sqrt{G}}{\sigma_e \sigma_\omega} (2m+1) - \frac{\sigma_\omega^2 \ell^2}{2}\right]$

Gain is reduced when electron beam duration σ_e approaches the inverse bandwidth of crystal $1/\sigma_{\omega}$

⁺ G. Dattoli, G. Marino, A. Renieri, and F. Romanelli, *IEEE J. Quantum Electron.* **17**, 1371 (1981); P. Elleaume, *IEEE J. Quantum Electron.* **21**, 1012 (1985)

Longitudinal dynamics of an XFELO: Supermode decomposition of the radiation field

We decompose the growing radiation using the Hermite basis function, each of which grow according to their supermode growth rate:



R. R. Lindberg and K.-J. Kim, Phys. Rev. ST-Accel. Beams 12, 070702 (2009)

Longitudinal dynamics of an XFELO: GINGER (2D FEL code) simulation



 10^{2}

100

10-

10

0

50

100

150

200

Energy (µJ)

Nonlinear saturation and steady state operation

- Particle trapping leads to a nonlinear reduction of the FEL gain when $P_{\text{FEL}} \sim (\gamma mc^2)/N_u = P_{\text{beam}}/N_u$
- This corresponds to the field amplitude for which an average electron makes ~1/2 oscillation in the potential generated by the radiation
- Alternatively, this as the field amplitude for which an electron changes its scaled energy by an amount of order the FEL bandwidth $1/N_u$

- Steady-state is reached when the (saturated) FEL gain balances the cavity losses
- In ideal scenario, we expect the fluctuation level to be of order the inverse amplification up to saturation, $P_{\rm noise}/P_{\rm FEL} \lesssim 10^{-5}$
- In simulations we often find $P_{\text{noise}}/P_{\text{FEL}} < 10^{-3}$, but sometimes not (more on this near the end...)





XFELO operating at a harmonic of the fundamental can significantly decrease electron beam energy[†]

- Madey's theorem says that in the low-gain limit $G_h \propto \frac{\partial}{\partial \omega} S_{\text{spont}}(\omega)$, and it turns out that gain can be larger at higher harmonics (fixed e-beam energy, number of undulator periods, etc.)
- This conclusion applies if the energy spread is sufficiently small:

 $h \frac{\sigma_{\gamma}}{\gamma} \lesssim \frac{1}{2\pi N_u}$ Variation of the resonance energy at harmonic *h* must be small

- For an XFELO, this typically means that $\Delta \gamma / \gamma < 2 \times 10^{-4} / h$
- Harmonic lasing may make an XFELO possible with low charge operation at the 4 GeV superconducting linac planned for LCLS-II§



[†] J. Dai, H. Deng, Z. Dai, *Phys Rev. Lett.* **108**, 034802 (2012) § T. Maxwell and J. Hastings, private communication

Optimization of LCLS-II electron beam profile



W. Qin (Peking), Y. Ding, K. Bane, et al. (SLAC)

Electron beams by design

- We're faced with a common problem in accelerator physics: Find a set of inputs that result in desired performance subject to certain constraints INPUTS: Photocathode laser, beamline elements, grating "dechirper," ...
 OUTPUTS: Peak current, emittance, energy spread, mean energy and angle, ...
 CONSTRAINTS: Total charge, laser power, heating loads on SRF and "dechirper," ...
- Present optimization involves a fairly intense simulation effort using genetic algorithms that are guided by ingenuity and experience⁺
- Similar genetic algorithms are commonly applied to other optimization problems in accelerator physics[§]
- BUT, genetic algorithms tend to be numerically intensive and furthermore seem to be disfavored by most optimization specialists
- What other optimization methods might be suitable?
- Does viewing this particular optimization as an "inverse problem" help?
- How do we insure that the optimized design is robust?

[†] W. Qin (Peking), Y. Ding, K. Bane, and other SLAC collaborators

§ e.g. M. Borland, V. Sajaev, L. Emery, and A. Xiao, Proc. of the 2009 Particle Accel. Conf. p. 3851, L. Yang, Y. Li, W. Guo, and S. Krinsky, Phys. Rev. ST-Accel. Beams 14, 054001 (2011).

X-ray cavity configurations



[†] K.M.J. Cotterill, Appl. Phys. Lett. **12**, 403 (1968) K.-J. Kim and Yu. Shvyd'ko, Phys. Rev. ST-AB 12, 030703 (2009)

Cavity stabilization proof of principle

To preserve radiation-electron beam overlap and FEL gain, we require:

- 1. Cavity length stability $\delta L < 3 \mu m$ (relatively easy)
- 2. Crystal angular stability $\delta\theta \sim$ 10 nrad (less straightforward)





Crystal stability of \sim 15 nrad rms was shown at the APS HERIX monochromator

Stoupin, Lenkszus, Laird, Goetze, Kim, and Shvyd'ko, Rev. Sci. Instrum. 81, 055108 (2010)

Beryllium compound refractive lens test @ APS



- 1. Transmission of Beryllium CRL with f = 50 m was measured to be ~99%
- 2. Wavefront measurement data shows < 1 micron surface errors



3. The resulting wavefront distortions should not negatively impact FEL gain, but their precise effect on FEL output has not yet been determined

Measurements by S. Stoupin, J. Kryziwinski, T. Kolodziej, Y. Shvyd'ko, D. Shu, X. Shi

Effect of imperfections and fluctuations on steadystate XFELO output

Requirements on stability to maintain FEL gain are relatively easy to specify

Electron beam arrival time << bunch length

Angular deviation of x-rays due to cavity Angular deviation of electron bunch << Divergence of the FEL mode whose $\sigma_{x'} \sim (\lambda/N_u)^{\frac{1}{2}} \sim \text{few} \times 10^{-7}$

 Fluctuations that occur on time scales much less than the cavity ring-down time are averaged over to reduce gain

(e.g., fast energy variations ≈ increase in energy spread)

 Fluctuations that occur on time scales much longer than the cavity ring-down time result in variations of the x-ray output

(e.g., slow energy variations lead to slow changes in photon energy)

- How do these fluctuations affect the details of the x-ray output?
 - Massive simulation effort is relatively straightforward but rather inelegant
 - Is there an approach that is more sophisticated then the previous simple arguments but less onerous then a full-blown simulation?

Ultimate stability of XFELO output

- The energy fluctuations in the FEL mode should be $\sim P_{\rm noise}/P_{\rm FEL}$ < 10^{-4}
- For some parameters, XFELO simulations show power oscillations at steady-state saturation



- Larger amplitude oscillations have been observed in long-wavelength FEL oscillators⁺
 - Limit-cycle type behavior associated with gain fluctuations whose bandwidth $\sim 1/N_u$
 - XFELO Bragg crystals should filter out this behavior since $\sigma_{\omega}/\omega \ll 1/N_{u}$
- Is the difference a numerical artifact, or indicative of other relevant physics?
- Either way, stability should be determined by that of the underlying nonlinear map
- Can we develop a reliable, useful model of non-linear saturation?
 - Perhaps building upon quasilinear theory[§], phenomenological models of gain saturation^x, statistical mechanical analyses[‡], and/or analysis of a model nonlinear map associated with an FEL oscillator[¥]...

⁺ B.A. Richman, J.M.J. Madey, E. Szarmes, *Phys. Rev. Lett.* **63**, 1682 (1989)

§ N. A. Vinokurov, Z. Huang, O. A. Shevchenko, and K.-J. Kim, *NIMA*. **475**, 74 (2001) ‡ P. de Buyl, D. Fanelli, R. Bachelard, G. De Ninno, *PRST-AB* **12**, 060704 (2009) ¤ G. Dattoli, S. Cabrini, and L. Giannessi *Phys. Rev. A* 44, 8433 (1991)
 ¥ T. M. Antonsen Jr. and B. Levush, *Phys. Fluids B* 1, 1097 (1989)

Ryan Lindberg – FEL Oscillator – IPAM Beam Dynamics Workshop, Jan. 2017

XFELO 2

0.1 ps

400 A

1000

14.4 keV

Frequency stabilized, mode-locked XFELO



- Total bandwidth set by pulse duration ~1/Δt
- Mode spacing set by periodicity 1/T_{period}
- Mode spectral width set by number of pulses 1/NT_{period}

Relies on phase coherence across all pulses

Can we stabilize the cavity to less than a wavelength and do this for an XFELO?



Does phase coherence persist in the presence of other imperfections/fluctuations?

Conclusions

- An x-ray FEL oscillator is a complementary source to SASE FELs:
 - An XFELO is a stable, fully coherent x-ray source with ultra-low spectral bandwidth
 - An XFELO has significantly fewer photons/pulse than SASE, but comparable brightness
- We have a firm handle on the linear XFELO physics, and find good agreement between theoretical calculations and detailed FEL simulations understand
 - This has clarified potential of XFELOs lasing at higher harmonics
- Successful e-beam optimization methods have been applied to the XFELO, but are there more efficient techniques?
- Most of the XFELO enabling technologies are available, and we need to incorporate these "real world" effects more completely into XFELO theory and simulation
- We understand the basic phenomena of non-linear saturation and approach to steady-state operation, but lack a more detailed theoretical model
 - Better grasp on the role of errors and fluctuations on the x-ray output, particularly for advanced applications like frequency comb generation
 - Provide theoretical guidance on ultimate stability for different XFELO parameters
- Ultimately, we can characterize XFELO performance with a dedicated simulation effort, but would prefer to have better theoretical tools to direct and distill this effort