Signatures of misalignment in x-ray cavities of cavity-based x-ray free-electron lasers

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Cavity-based x-ray free-electron lasers (CBXFEL) will allow use of optical cavity feedback to support generation of fully coherent x-rays of high brilliance and stability by electrons in undulators. CBXFEL optical cavities comprise Bragg-reflecting flat crystal mirrors, which ensure x-rays circulation on a closed orbit, and x-ray refractive lenses, which stabilize the orbit and refocus the x-rays back on the electrons in the undulator. Depending on the cavity design, there are tens of degrees of freedom of the optical elements, which can never be perfectly aligned. Here, we study signatures of misalignment of the optical components and of the undulator source with the purposes of understanding the effects of misalignment on x-ray beam dynamics, understanding misalignment tolerances, and developing cavity alignment procedures. Betatron oscillations of the x-ray beam trajectory (both symmetric and asymmetric) are one of the characteristic signatures of cavity misalignment. The oscillation period is in the general case a non-integer number of round-trip passes of x-rays in the cavity. This period (unlike the amplitude and offset of the oscillations) is independent of the type of misalignment and is defined by cavity parameters. The studies are performed on an example of a four-crystal rectangular cavity using analytical and numerical wave optics as well as ray-tracing techniques. Both confocal and generic stable cavity types are studied.

I. INTRODUCTION

The next generation of hard x-ray free-electron lasers (XFELs) operating in a high-repetition-rate (\(\simeq\) MHz) pulse sequence mode \cite{1, 2} will allow for optical cavity–based feedback, like in classical lasers \cite{3}. Unlike self-amplified spontaneous emission (SASE) XFELs \cite{4–6}, the new cavity-based XFELs (CBXFEL) \cite{7, 8} are capable of generating fully coherent x-ray beams of high brilliance and stability. Two major CBXFEL schemes are presently considered: low gain and high gain.

An x-ray free-electron laser oscillator (XFELO) \cite{8–12} is a low-gain CBXFEL, which requires a low-loss (high-Q) x-ray cavity. XFELOs are promising to generate radiation of unprecedented spectral purity with a meV bandwidth.

Another possible realization of the CBXFEL is a high-gain regenerative amplifier free-electron laser (XRAFEL) \cite{7, 13–15}, which can reach saturation after a few round-trip passes. It can therefore allow for a high (close to 100\%) extraction efficiency. It can use a similar or identical cavity as an XFELO; but, with substantially relaxed tolerances on the efficiency and stability.

Classical laser oscillator cavities in the optical domain are typically composed of two curved high-reflectance backscattering mirrors, each ensuring laser beam circulation, refocusing, and stabilization \cite{3}. In the hard x-ray domain, these functions have to be assigned to two different types of optical elements \cite{8, 9}: high-reflectance flat Bragg-reflecting diamond crystal mirrors \cite{16, 17} and x-ray–transparent beryllium refractive paraboloidal lenses \cite{18, 19}. Different cavity designs have been considered: fixed-photon-energy two-crystal cavity \cite{8, 9, 20}, tunable-photon-energy four-crystal cavity \cite{9, 21}, and tunable compact non-planar six-crystal cavity \cite{22}.

Here, we are considering as an example a fixed-photon-energy four-crystal rectangular cavity proposed for a joint Argonne National Laboratory (ANL) and SLAC National Laboratory (SLAC) CBXFEL R&D project \cite{23}. A CBXFEL with a rectangular cavity is presented in Fig. 1. It is composed of an undulator x-ray source and a cavity comprising four Bragg-reflecting flat-crystal mirrors \(C_1\), \(C_2\), \(C_3\), and \(C_4\), along with two refractive lenses (\(L_1\) and \(L_2\)) as focusing elements. The limited space in the Linac Coherent Light Source (LCLS) undulator tunnel \cite{2} determines the choice of the fixed-photon-energy rectangular cavity versus a tunable bow tie–type four-crystal cavity \cite{9}. In the future, the rectangular cavity could be upgraded to a tunable non-planar six-crystal cavity \cite{22} taking the same footprint.

There are tens of degrees of freedom of the optical elements (depending on the cavity design)—many more than in a classical laser oscillator. All of them have to be aligned with a precision ensuring that the to-be-amplified x-ray beam returning into the undulator (after traveling tens to hundreds of meters in the cavity and being refocused to a spot of a few tens of microns) meets a fresh electron bunch of a similar size and a few tens of microns in length. Cavity alignment is one of the major challenges in the realization of CBXFELs. To this end, several essential questions have to be addressed, in particular: (i) What are the typical misalignment pat-
FIG. 1: Schematic of a cavity-based XFEL with an undulator x-ray source together with a four-crystal (C₁-C₄), two-lens (L₁-L₂) rectangular x-ray cavity and x-ray diagnostics [23]. Cavity round-trip length $2(L + W) \approx 65$ m. X-ray diagnostics tools include x-ray beam intensity monitors (XBIMs) and an x-ray beam position, profile, and intensity monitor (XBPM).

terns? (ii) Can they be identified with x-ray beam monitors? (iii) Can different degrees of freedom be disentangled and the number of mutually dependent degrees of freedom reduced? (iv) What are the misalignment tolerances? (v) How can the cavity be aligned?

In the first step of our analysis to address these questions, we are studying the spatial, angular, and temporal behavior of x-rays in the rectangular x-ray cavity using analytical tools developed for classical laser oscillator cavities [3, 24]. These methods have also been applied to study statistical misalignment tolerances in CBXFEL cavities [10, 23, 25]. We are using matrix ray tracing, paraxial resonator theory, and Gaussian mode theory to derive stable, self-consistent solutions for the Gaussian beams in the cavity; to determine cavity parameters; and to analyze beam instabilities in both a perfectly aligned cavity and a cavity with misaligned optical components.

Although in general this analytical approach is quite powerful, it has limitation, because the Bragg-reflecting crystal mirrors are treated as 100%-reflecting mirrors with unrestricted spectral and angular reflection widths. In the second step of our analysis, we address this limitation by using numerical simulation tools, which involve calculations based on the dynamical theory of Bragg diffraction of x-rays in crystals [26]. With these tools, we are able to take the actual properties of the optical elements into account.

The short-term goal of these studies is to understand the spatial, angular, and temporal behavior of x-rays and the response of the cavity x-ray monitors to typical misalignment patterns of x-ray optical components and of the x-ray source, with a view to developing human-controlled cavity alignment procedures. The long-term goal is to develop computer-assisted algorithms (e.g., utilizing machine learning) to guide cavity alignment.

We note, that our studies are limited to empty cavity conditions. XFEL gain effects, in particular, gain guiding effects typical for XRAFEL are not considered here.

The paper is organized as follows. Section II covers the function and optical design of the rectangular cavity and its parameters. Results of analytical studies of the x-ray cavity are presented in Section III, and results of numerical simulation studies are given in Section IV. A strategy for cavity alignment is presented in Section V. Conclusions and outlook are discussed in Section VI.

II. FOUR-CRYSTAL RECTANGULAR CAVITY OPTICAL DESIGN AND PARAMETERS

Figure 1 shows the schematic of the CBXFEL [23] with the rectangular x-ray cavity studied here. Parameters of the x-ray cavity, x-ray source, and optical components are listed in Table I and explained below.

X-rays from an undulator source propagate through the x-ray cavity composed of four Bragg-reflecting crystal mirrors C₁-C₄ and two focusing lenses L₁-L₂. In the perfectly aligned cavity, the optical axis is a rectangle having sides $L$ and $W$ ($L > W$), with crystals placed in its corners, while the lenses are placed in the symmetry points at distances $\ell/4$ from the source, where $\ell = 2(L + W)$ is the round-trip length. Different locations of the lenses could be considered as well, but only this symmetric configuration is studied here.

The crystal mirrors compose two backscattering units, which bracket the undulator, with two crystals C₁ and C₄ on one end of the undulator and two crystals C₂ and C₃ on the other end. In each unit, two successive Bragg reflections reverse the direction of the beam, which fixes the incidence and reflection angles to exactly $45^\circ$. This geometry requires an x-ray source generating photons with a $\sigma$-polarization component (electric field vector perpendicular to the cavity plane). Diamond crystals are chosen as Bragg reflecting crystal mirrors because of their high reflectivity, x-ray transparency, and resilience [17]. In particular, the 400 Bragg reflection from diamond crystal is used, a choice dictated by the practical consideration that it is easier to obtain high-quality diamond crystal plates in the 100 orientation than in other orientations [27]. The 400 Bragg reflection with $45^\circ$ incidence angle predefines a 9.83102-keV central photon energy of the cavity and of the x-ray source, assuming
TABLE I: Parameters of the rectangular cavity, x-ray source, and optical components [23] used in the calculations presented in the paper. Parameters marked with asterisk are derived from other parameters of the table.

| Parameters | Values |
|------------|--------|
| Cavity     |        |
| Type       | rectangular |
| Length L   | 32 m |
| Width W    | 0.65 m |
| Round-trip length τ = L/c | 65.3 m |
| Round-trip time τ = L/c | 218 ns |
| Source     |        |
| Type       | Gaussian beam |
| Rayleigh length* Zσ* | 25.67 m |
| Transverse size* σx,y* (rms) | 15.9 μm |
| Angular size* σx,y* (rms) | 0.62 μrad |
| Central photon energy* E(θ) | 9.83102 keV |
| Spectral bandwidth (as used in numeric simulations) | 100 meV |
| Crystals C1-C4 | Material |
| Bragg reflection | Diamond (400) |
| Central angle of incidence θ | 45° |
| Thickness | C1: 20 μm; C2-C4: 500 μm |
| Temperature | 300 K |
| Spectral reflection width ΔE | 90 meV |
| Angular reflection width Δθ | 9 μrad |
| Lenses L1-L2 | Material |
| Lens type | Beryllium Paraboloidal 2D |
| Focal length f(1) = ℓ/4 | 16.3 m |
| f(2) = ℓ/8 + 2Zσ*2/ℓ | 28.3 m |
| Radius of curvature R(1) | 115 μm |
| R(2) | 200 μm |

all crystals operate at the same temperature of 300 K. Crystals C2-C4 are assumed to be 500 μm thick for high reflectivity and mechanical stiffness. Crystal C1 is assumed to be 20 μm thick for output coupling of ≃3% of the interactivity power [8, 9, 28].

The x-ray source is assumed to generate a Gaussian beam with a Rayleigh length Zσ* matched to the electron beam beta function at the undulator center [23], which is considered to be the cavity origin with z = 0. The Rayleigh length and photon wavelength λ = hc/E define the root mean square (rms) x-ray source (Gaussian beam waist) transverse size σx,y* = √(λ/4π)Zσ*, and the rms angular source divergence σx,y* = √(λ/4π)Zσ*. The spectral bandwidth of the source is limited artificially in these calculations to 100 meV to reduce computation time and to match the spectral width of the Bragg reflections ΔE = 90 meV.

The focal length f of the focusing elements L1-L2 has to be properly chosen in order for the Gaussian beam with Rayleigh length Zσ* to be a stable and self-consistent (self-reproducing after each round trip) cavity mode, as discussed in Section III, Eq. (5). The focal length values − f(1) and f(2) for confocal and generic cavities, respectively (Table I) − were chosen based on this consideration but also for the following practical reason.

We chose beryllium paraboloidal lenses [18] as x-ray focusing elements in the cavity. They are manufactured with discrete values of the radius of curvature R [29]. For the photon energy in question, the lens with R = 200 μm has a focal length of f(2) = 28.3 m, close to (but not exactly) the value required to maintain a cavity mode with the desired properties. In the following calculations, we use this value for f(2) in the generic cavity and adjust appropriately the values of Zσ*, σx,y*, and σx,y*, as listed in Table I. The same Zσ*, σx,y*, and σx,y* values are used for the confocal cavity with f(1) = ℓ/4 = 16.3 m.

In our studies, x-ray beam size, position, angle, and intensity are calculated and “monitored” every round-trip pass in the undulator center and in the midpoint between crystals C1 and C4. In an experiment, non-invasive x-ray beam position, profile, and intensity monitors (XBPMs) installed in these locations can provide all these values except the beam angle. To monitor x-ray beam angles at different locations in the cavity, x-ray beam intensity monitors (XBIM) D1-D4 can be used to measure the intensity of x-rays penetrating through the diamond crystals on each round-trip pass (see Fig. 1). A high level of transmitted intensity would signal that the angle of incidence of x-rays to the (400) reflecting crystal planes is far off the peak reflectivity angle. For this reason, we calculate in our studies the intensity of the x-rays transmitted through crystals C1-C4.

The optical axis of the cavity is defined along the trajectory of x-rays in the perfectly aligned cavity. We use local right-handed reference coordinate systems, which propagate with the z-axis always along the optical axis, the y-axis perpendicular to the optical axis, and the x-axis parallel to the cavity plane, and x × y = z, as indicated in Fig. 1. The optical elements inherit the same coordinate system as the incident rays. For angular variation of the ray slope in the (x, z) plane and for rotation of the optical elements, the counterclockwise sense is defined as positive.

III. ANALYTICAL STUDIES

Here, we are using the paraxial ray-transfer matrix technique and paraxial wave optics to propagate x-rays and Gaussian beams through the optical elements of the cavity shown in Fig. 1, to determine parameters of the stable cavity and the self-consistent Gaussian beam.
modes and to analyze cavity instabilities due to the x-ray source and misalignment of optical elements in the cavity plane.

A. Stable and self-consistent solution for a perfect cavity

A paraxial ray in any reference plane perpendicular to the optical axis is given by its distance \( x \) from the optical axis and by its angle \( x' \ll 1 \) with respect to the axis. A ray vector \( r_0 = \left[ x_0 \ y_0 \right] \) at the source (or input) plane is transformed to \( r_1 = \hat{O} r_0 \) at the image (or output) plane, where \( \hat{O} = \{AB;CD\} \) is a \( 2 \times 2 \) ray-transfer matrix of an optical element placed between the planes.

The ray-transfer matrix of the cavity is a sequential product of three discrete ray-transfer matrices: propagation in free space \( \hat{P}(l) \) over distance \( l \), reflection from a crystal mirror \( \hat{C} \), and focusing by lens \( \hat{L}(f) \) with focal length \( f \), which are given by

\[
\hat{P}(l) = \begin{bmatrix} 1 & l \\ 0 & 1 \end{bmatrix}, \quad \hat{C} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \hat{L}(f) = \begin{bmatrix} 1 & 0 \\ -1/f & 1 \end{bmatrix},
\]

respectively [3, 24, 30]. The only impact of the crystal mirror is the inversion of the ray vector space and angular coordinates [31]. The finite angular and spectral acceptance of the Bragg-reflecting crystal mirrors are not taken into account within this approach but will be included in the numerical simulations approach in Section IV.

The ray-transfer matrix of the cavity in Fig. 1 with four crystals and two lenses is calculated as a product \( \hat{R} = \hat{P}(\ell/2)\hat{C}\hat{P}(W_\ell)\hat{L}(f)\hat{P}(\ell/2)\hat{C}\hat{P}(L)\hat{C}\hat{P}(W_\ell)\hat{L}(f)\hat{P}(\ell/2)\hat{C}\hat{P}(\ell/4) \). The source ray vector \( r_0 \) at the undulator center (considered to be the cavity origin, with \( z = 0 \)) is transformed by this matrix to the image ray vector \( r_1 \) at the same location after the round trip. Because \( \hat{C} = -\hat{I} \), where \( \hat{I} = \{10;01\} \) is the unit matrix, the ray-transfer matrix of the cavity simplifies to \( \hat{R} = \hat{P}(\ell/4)\hat{L}(f)\hat{P}(\ell/2)\hat{L}(f)\hat{P}(\ell/4) \) and becomes

\[
\hat{R} = \begin{bmatrix} \frac{8f(f-\ell)+\ell^2}{8f^2} & \frac{\ell(32f^2-12f\ell+\ell^2)}{32f^2} \\ \frac{8f(f-\ell)+\ell^2}{8f^2} & \frac{8f(f-\ell)+\ell^2}{8f^2} \end{bmatrix},
\]

using Eq. (1). The equivalent scheme of the unfolded symmetric cavity is shown in Fig. 2.

The cavity is stable (meaning a paraxial ray within the cavity does not escape after numerous passes) when the matrix trace \( (A + D) \) obeys the inequality \(-1 \leq (A + D)/2 \leq 1 \) [3, 24]. In our particular case, stability requires \( f \geq \ell/8 \), which is a relaxed condition.

We now use the calculated cavity ray-transfer matrix (2) to determine self-consistent Gaussian beam modes in the cavity, i.e., the modes self-reproducing after each round trip. Knowledge of the ray-transfer matrix of an optical system is particularly useful as it also describes the propagation of the Gaussian beams through the system [3, 24]. Gaussian beams are eigenstates of paraxial wavefields in free space, and they can be eigenstates of the linear optical systems presented by ABCD ray-tracing matrices.

The self-consistent solutions can be found by applying the ABCD propagation law: a Gaussian beam with the complex beam parameter \( q_0(z) = Z + iZ_o \) in the source reference plane 0 (here \( Z_o \) is the Rayleigh range) is transformed to a Gaussian beam with the beam parameter

\[
q_1 = \frac{Aq_0 + B}{Cq_0 + D} \quad (3)
\]

in reference plane 1 (image plane). We assume here that the waist of the Gaussian beam source is at the undulator center with \( z = 0 \) and therefore \( q_0 = iZ_o \).

A mode with the complex beam parameter \( q_0 \) is a self-consistent cavity mode if after the complete round trip of the beam it returns to its initial value, i.e.,

\[
q_1 = q_0 = iZ_o \quad (4)
\]

Combining Eqs. (2)-(4), we arrive at a second-order equation in \( Z_o^2 \) for the self-consistent Gaussian mode containing the focal length \( f \) of the lenses and the cavity round-trip length \( \ell \) as parameters. Alternatively, the equation can be solved for the focal length \( f \) required for a specific self-consistent value of \( Z_o^2 \). There are two possible solutions:

\[
f^{(1)} = \frac{\ell}{4}, \quad f^{(2)} = \frac{\ell}{8} + \frac{2Z_o^2}{\ell} \quad (5)
\]

In both cases \( f \geq \ell/8 \) and therefore both represent stable solutions. We note that \( f^{(2)} = f^{(1)} \), provided \( Z_o = \ell/4 \). We next analyze the beam dynamics for each solution.

1. Self-consistent confocal cavity solution

A Gaussian beam with any Rayleigh range \( Z_o \) is a self-consistent solution if the relationship \( f^{(1)} = \ell/4 \) of Eq. (5) is fulfilled. This relationship corresponds to a confocal symmetric stable laser cavity [3, 24], in which the focal points of both lenses coincide with each other, with the cavity origin (at the undulator center), and with the midpoint on the return path.

Any Gaussian beam of Rayleigh range \( Z_o \) and beam waist of rms width \( \sigma_o = \sqrt{\lambda Z_o/4\pi} \) located at the cavity
origin (which is also a focal point of lens $L_1$) is refocused by lens $L_1$ into a Gaussian beam of Rayleigh length $Z_1 = Z_o M^2$ with beam waist of rms width $\sigma_1 = M \sigma_o$ located at the second focal point of lens $L_1$ (which is also the midpoint of the return path). Here

$$M = f(1)/Z_o = \ell/4Z_o$$

(6)
is the absolute value of the magnification factor (see Section 3.2 of [30]). The location of the second Gaussian beam waist is in the focal point of the second lens $L_2$. As a result, this Gaussian beam is refocused with magnification $1/M$ by the second lens $L_2$ to a Gaussian beam with the waist located at the cavity origin (the second focal point of lens $L_2$), and with exactly the same Rayleigh length and rms width as the original beam. In the particular case of $Z_o = f_o = \ell/4$, magnification $M = 1$ results in the same Rayleigh length $Z_1 = Z_o$ and beam width $\sigma_1 = \sigma_o$ at the cavity midpoint as well as at the cavity origin. Figure 3 shows appropriate beam profiles with different magnification $M$.

The ABCD cavity matrix given by Eq. (2) reduces in the confocal cavity case to a very simple

$$\hat{R}^{(1)} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} = -\hat{I}.$$  

(7)
The $n$-pass confocal cavity matrix can be immediately calculated as $[\hat{R}^{(1)}]^n = (-1)^n \hat{I}$, which in turn allows us to calculate the transformation of an arbitrary initial source ray $r_o$ at the cavity origin after $n$ passes:

$$r_n = [\hat{R}^{(1)}]^n r_o = (-1)^n r_o.$$  

(8)

For an x-ray beam with a distribution of source rays characterized by an initial average ray vector $\bar{r}_o$ that represents the offset of the beam from the optical axis, Eq. (8) also describes the pass-to-pass variation of the beam position $\bar{r}_n = (-1)^n \bar{r}_o$ at the source location. The beam position changes periodically but is reproduced every second pass. If there is no initial beam offset, i.e., $\bar{r}_n = 0$, the beam position is reproduced (is self-consistent) every pass. In contrast, the beam size

$$\sigma_n = \sqrt{(x_{n} - x_o)^2} = \sqrt{\frac{x_n - x_o}{Z_o}} = \sigma_o$$

(9)
ever changes at the source origin in the confocal cavity.

2. Self-consistent generic cavity solution

The second solution to Eq. (5) represents a generic cavity configuration. A Gaussian beam with any Rayleigh length $Z_o$ is a valid self-consistent stable solution if focal length $f(2)$ obeys Eq. (5). For this case, the magnification factor is always $M = 1$ for any $Z_o$ (see Section 3.2 of [30]). The second waist is located at the midpoint of the return path and has the same beam waist size as the original Gaussian beam, as shown schematically in Fig. 3 for $M = 1$.

The cavity ray-transfer matrix Eq. (2) in this case is

$$\hat{R}^{(2)} = \begin{bmatrix} \frac{1 - 96r^2 + 256r^4}{(16r^2 + 1)^2} & \frac{\ell(256r^4 - 16r^2)}{(16r^2 + 1)^2} \\ \frac{16 - 256r^2}{(16r^2 + 1)^2} \end{bmatrix}, \quad r = Z_o/\ell,$$

(10)

which transforms to

$$\hat{R}^{(2)} = \begin{bmatrix} \cos \phi Z_o \sin \phi \\ -(1/Z_o) \sin \phi \cos \phi \end{bmatrix},$$

(11)

using a new parameter $\phi$ defined as

$$\cos \phi = A = \frac{1 - 96r^2 + 256r^4}{(16r^2 + 1)^2},$$

(12)
$$\sin \phi = B/Z_o = -CZ_o = \frac{16(16r^2 - 1)}{(16r^2 + 1)^2},$$

(13)
$$\phi = 4 \arctan(1/4r).$$

(14)

Phase $\phi$ is the accumulated within one round trip Gouy phase $\arctan(z/Z_o)$ of the Gaussian beams [32]. With the cavity parameters provided in Table I,

$$\phi = 2\pi/2.76.$$  

(15)

Using Eq. (11), a ray-transfer matrix of a multi-pass cavity can be calculated as

$$[\hat{R}^{(2)}(\phi)]^n = \begin{bmatrix} \cos \phi n & Z_o \sin \phi n \\ -(1/Z_o) \sin \phi n \cos \phi n \end{bmatrix},$$

(16)

where $n$ is a number of passes. This expression in turn allows us to calculate how an arbitrary initial source ray $r_o$ at the cavity origin changes after $n$ passes:

$$r_n = [\hat{R}^{(2)}(\phi)]^n r_o = \begin{bmatrix} x_o \cos \phi n + x_o' Z_o \sin \phi n \\ x_o' \cos \phi n - (x_o/Z_o) \sin \phi n \end{bmatrix}.$$  

(17)

We now consider a beam of rays with non-zero average distribution of the initial spatial $\bar{x}_o$ and initial angular $\bar{x}_o'$ offset from the optical axis. From Eq. (17) it
follows that the average spatial and angular beam positions at the cavity origin oscillate after each round-trip pass as
\[
\bar{\mathbf{r}} = \begin{bmatrix} \bar{x}_n \\ \bar{x}_n' \end{bmatrix} = \begin{bmatrix} x_0 \cos \phi n + x_0' Z_n \sin \phi n \\ x_0' \cos \phi n - (x_0/Z_n) \sin \phi n \end{bmatrix},
\]
with a period \(2\pi/\phi\), which is a non-integer number of round trips in the general case. We will refer to this effect as betatron oscillations of x-rays in a cavity, by analogy to similar effects in periodic accelerator structures [33]. This effect is of course typical of laser cavities as well [3]. The importance of the betatron oscillations for a closed optical cavity was pointed out recently [25]. The phase \(\phi\) corresponds to the phase advance of the betatron oscillations with each round-trip pass.

Note that, from Eq. (18), betatron oscillations are absent if the initial beam (source) is perfectly aligned with the optical axis (i.e., \(\bar{x}_0 = 0\) and \(\bar{x}_0' = 0\)). The presence of the betatron oscillations thus indicates a misaligned source. Table II shows an example of non-zero beta-oscillation amplitudes at the cavity origin oscillate after each round-trip. The equivalence of the paraxial Gaussian ray and Gaussian wave optics, which is well established [3, 24, 25], justifies using ray-transfer techniques to study other aspects of cavity performance, in particular for a cavity with misaligned optical components (Section IV).

**TABLE II: Initial x-ray beam (source) alignment errors and subsequent spatial and angular beam betatron oscillation amplitudes calculated with Eq. (18).**

| Initial alignment errors \(\bar{x}_0, \bar{x}_0'\) amplitude | \(\bar{x}_0, \bar{x}_0'\) amplitude |
|-----------------------------------------------------------|----------------------------------|
| \(\bar{x}_0 = 0, \bar{x}_0' = 200 \text{ nrad}\) | \(\bar{x}_0 = 5 \text{ \(\mu\)m}, \bar{x}_0' = 0\) |
| \(\bar{x}_0 = 5 \text{ \(\mu\)m}, \bar{x}_0' = 0\) | \(\bar{x}_0 = 5 \text{ \(\mu\)m}, \bar{x}_0' = 200 \text{ nrad}\) |

valid also for a misaligned source. It is similar to the case of the self-consistent solution for Gaussian beams given by Eq. (4).

Remarkably, according to Eq. (22), this stable solution is valid only if the x-ray spatial and angular source sizes \(\sigma_{x_0}\) and \(\sigma_{x_0'}\), respectively, obey the same relationship as those of the Gaussian beam with Rayleigh range \(Z_n\) at its waist location.

In all other cases, when \(S \neq 1\), the beam size and angular spread oscillate periodically from pass to pass with a twice smaller period around average values that can be smaller or larger than the initial beam size values, depending on the \(|S|^2\) value.

This result implies that the ABCD ray-transfer matrix propagates a collection of rays with a Gaussian distribution of position and angles given by Eq. (22), exactly in the same way as it propagates the Gaussian beam with Rayleigh range \(Z_n\). The equivalence of the paraxial Gaussian ray and Gaussian wave optics, which is well established [3, 24, 25], justifies using ray-transfer techniques to study other aspects of cavity performance, in particular for a cavity with misaligned optical components (Section IV).

### B. Ray optics with misaligned elements

The ray-transfer matrix approach can also be used to propagate rays through optical systems with misaligned optical elements [3]. Here, we calculate how the rays are transformed in such cases. These results will be applied in Section IV to calculate x-ray trajectories in a cavity with misaligned elements. Those trajectories will be compared with results obtained with a more advanced numerical simulations approach, which uses the x-ray optics modeling package Shadow3 [34].

Figure 4 illustrates the relationships used in calculating misalignment. Suppose an optical element (a crystal or a lens) is displaced from the perfect configuration by a distance \(\xi\) and an angle \(\delta\). The distorted propagation of the x-rays can be calculated by (i) displacing the incident x-rays by the same amount as the optical element but in the opposite direction \((-\xi\) and \(-\delta\)), (ii) transferring the ray with a standard matrix \([\hat{C} \text{ or } \hat{L}(f)]\), and (iii) moving the transferred ray back by the adjusted amount. As a result, the coordinates of the distorted ray are given by

\[
\begin{bmatrix} x_n \\ x_n' \end{bmatrix} = M \left( \begin{bmatrix} x_{n-1} \\ x_{n-1}' \end{bmatrix} - \begin{bmatrix} \xi \\ \delta \end{bmatrix} \right) + \begin{bmatrix} \xi \cos \gamma \\ \delta \end{bmatrix},
\]

where \(M\) is the standard ray-transfer matrix corresponding to the optical element \([\hat{C} \text{ or } \hat{L}(f)]\) and \(\gamma\) is the angle between the exit ray and the incident ray at the location of the optical element, as shown in Fig. 4. Note that the first adjustment of the ray position \((-\xi\) is relative to the incident ray. To restore the the exit ray to its correct position, it needs to be moved by the amount...
ξ \cos \gamma. For a crystal, the exit ray angle \( \gamma = 2\theta \) after crystal reflection with Bragg angle \( \theta \). For a lens, \( \gamma = 0 \).

Thus, the coordinates of the ray vector reflected by a misaligned crystal with a Bragg angle \( \theta = 45^\circ \) (corresponding to the case of our cavity) are

\[
\begin{bmatrix}
  x_n \\
  x_n'
\end{bmatrix}
= \hat{C}
\begin{bmatrix}
  x_{n-1} \\
  x_{n-1}'
\end{bmatrix}
+ \begin{bmatrix}
  \xi \\
  2\delta
\end{bmatrix},
\tag{25}
\]

and the coordinates after a misaligned lens are

\[
\begin{bmatrix}
  x_n \\
  x_n'
\end{bmatrix}
= L(f)
\begin{bmatrix}
  x_{n-1} \\
  x_{n-1}'
\end{bmatrix}
+ \begin{bmatrix}
  0 \\
  \xi/f
\end{bmatrix}.
\tag{26}
\]

Eq. (25) shows that crystal misalignment displaces the ray by an amount equal to the crystal’s positional displacement and deflects the ray by twice the crystal’s angular misalignment. Eq. (26) indicates that the ray propagation is not sensitive to angular misalignment of the lens and the angular deflection of the ray is proportional to positional displacement of the lens. Given the initial status of a ray and the misalignment status of the optical elements, the ray position and angle at locations of interest in the cavity can be traced, as will discussed in the next section.

## IV. NUMERICAL STUDIES

The paraxial ray-transfer matrix and wave-optics Gaussian beam approaches used in the previous section are limited because the cavity optical components—the crystals and lenses—are treated in simplified way. The Bragg-reflecting crystals are considered as 100%-reflecting flat mirrors with unrestricted spectral and angular reflection widths. Dynamical diffraction effects [26] are not taken into account. X-ray absorption in lenses, which limits their effective aperture [18], is also not considered. As a result, the round-trip losses in the cavity cannot be studied accurately.

We are using numerical simulation tools to provide for a more realistic account of the actual properties of the optical elements and to acquire more detailed insight into the spatial, angular, and temporal behavior of x-rays (x-ray beam dynamics) and the response of x-ray beam monitors to typical alignment errors.

The numerical simulations are performed in three dimensions, unlike the two-dimensional analytical studies performed in Section III.

In most cases, we consider the generic cavity, but we do examine the confocal cavity case in Section IV H for comparison.

### A. Method

Numerical simulations in this work are performed using the x-ray optics modeling package Shadow3 [34] in the Oasys environment [35, 36] and custom Python scripts.

As shown in Fig. 5, the simulation program starts with defining the x-ray source and all optical elements (crystals and refractive lenses) that exist in the cavity. The source generates x-rays with randomized positions, angles, and energies with a given Gaussian distribution. The rays propagate and interact with each optical element (OE) in the cavity and return to the source. When multiple-cycle simulation is desired, the x-ray beam keeps propagating and repeats similar simulations as in the first cycle. The status of all x-rays after each OE is recorded for the analysis.

In cases that are not affected by the limited reflection width of the crystals or by photoabsorption in lenses (e.g., for small spatial and angular beam deflections from the optical axes), the x-ray beam dynamics are also calculated, using the ray-tracing matrix approach (Section III B), and compared with the numerical simulation results obtained with the Shadow3 package.
The x-ray source and optical elements parameters of the simulated CBXFEL system are listed in Table I.

B. Perfectly aligned system

We commence with a perfectly aligned system and a generic cavity in which the optical elements and the x-rays source are in the spatial and angular positions shown in Fig. 1.

Figure 6 presents results of the numerical simulations, which will serve as a baseline to identify signatures of misalignment in subsequent studies. The graphs in the top four rows show variations after each round-trip cycle of the x-ray beam spatial position (a)-(b), angle (c)-(d), transverse beam size (e)-(f), and beam intensity (g)-(h) calculated either at the midpoint of the return path (left column) or at the x-ray source location (right column). The beam positions and angles are measured as a relative deviation of the average ray distribution from the optical axis. The beam size is calculated as the rms of the ray distribution.

Graphs (i)-(l) in the bottom row of Fig. 6 show the intensity (calculated for each cycle) of x-rays transmitted through crystals $C_1$-$C_4$, respectively. In an experiment, these intensities would be measured by the corresponding XBIMs $D_1$-$D_4$ shown in Fig. 1.

The analytical studies performed in Section III (for a perfectly aligned cavity with an x-ray source generating a self-consistent Gaussian beam) predict a perfectly reproducible beam after each round trip. In contrast, the numerical simulations show pass-to-pass periodic non-zero variation of the x-ray beam position, angle, and size in the perfectly aligned cavity at both source and midpoint. The x-ray beam trajectory oscillates with a period of 2.77 cavity cycles. This value corresponds exactly to the period of the betatron oscillations derived for a system with the same parameters featuring a perfectly aligned cavity but a misaligned source [see Eqs. (15), (17), and (18)].

As we noted in Section III, betatron oscillations are a signature of misalignment, in particular, of the x-ray source. We do in fact have a misaligned source in this case, but here the “misalignment” is an artifact arising from the use of a finite number of rays. Such a “beam” consisting of discrete rays is never perfectly aligned with the optical axis. Figure 6 provides a baseline for the scale of beam variations due to this artifact. In fact, the spatial and angular variations in Figs. 6(a)-(f) are very small, about 1/1000 of the beam size and angular beam divergence, and therefore can be neglected in this case.

To explore the scale of this artifact, we use simulations at two resolutions: $2 \times 10^5$ rays (red) and $2 \times 10^6$ rays (blue). Increasing the number of rays decreases the amplitudes of the oscillations, albeit at a cost of increased computation time, but they never reach zero (that would occur only with an infinite number of rays). The simulations of a misaligned cavity presented in the following sections use the lower resolution of $2 \times 10^5$ rays.

The beam size in Figs. 6(e)-(f) oscillates with a twice smaller period and an amplitude of $\sim 0.3 \mu m$ around an average value of $\sim 15.2 \mu m$. The oscillations are independent of the number of rays and therefore this effect is not the artifact discussed in the previous paragraph. The average beam size is smaller than the source size value of 15.9 $\mu m$ [See Table I]. According to Eqs. (19)-(21), this indicated that the numerical value of parameter $|S|^2 \neq 1$ [See Eq. (21)], i.e. x-ray source parameters are chosen slightly off those of a Gaussian beam with Rayleigh length $Z_o$ at its waist.

Figure 6 also shows the evolution of the beam intensity. The intra-cavity intensity of x-rays decays exponentially, with a half lifetime of $t_{1/2} = 10.8(1)$ cycles [see Figs. 6(g)-(h)]. We note that the faster decay during the first cycles occurs because the x-ray source bandwidth used in the calculations ($\sim 100 \text{ meV}$) is slightly larger than the $\sim 90 \text{ meV}$ bandwidth of the 400 Bragg reflection of the diamond crystals. The round-trip intensity losses are about 6.4%. Of this, $\sim 3 \%$ is coupled out through 20-$\mu m$-thick crystal $C_1$. Figure 6(i) shows the relevant out-coupling time dependence, with a decay
constant of 9.3 cycles. The remaining losses are due to photoabsorption in the lenses and crystals.

Figures 6(j)-(l) show the time dependence of leakage through crystals C_2-C_4, respectively, of x-rays belonging to the tails of the intra-cavity spectral distribution. The magnitudes of the signals are small, and they vanish rapidly as the tails become sharper after each Bragg reflection. If the crystal C_1 thickness is increased to match that of crystals C_2-C_4, the decay constant in Fig. 6(i) becomes as fast as those in Fig. 6(j)-(l).

C. Alignment errors

Having established the baseline performance for a perfectly aligned cavity, we now model the effects of typical angular and spatial alignment errors on the x-ray beam trajectory in the cavity and how these in turn are reflected in the temporal response of the beam monitors. In most cases, we consider alignment error of a single degree of freedom of a single optical component or of the x-ray source.

For example, one crystal in the cavity can be misaligned by yaw angle δ_c [crystal C_4 in Fig. 7(a)], which corresponds to the rotation around the ŷ_c-axis perpendicular to the crystal cavity, while the other crystals are aligned perfectly at the designed 45° to the optical axis and perpendicular to the cavity plane. Alternatively, the roll angle ρ of one crystal can be misaligned [crystal C_4 in Fig. 7(b)], corresponding to rotation around the axis formed by the intersection of the crystal surface and the cavity plane. A typical spatial alignment error ξ of crystal C_4 along the x̂_c-axis is shown in Figure 7(c). The arrows on the schematics show in all cases the positive direction of the alignment error.

Along with single-element alignment errors, we also consider a special multi-crystal error case, which we refer to as systematic angular misalignment. This kind of error is typical for fixed-photon-energy cavities, such as the four-crystal cavity we are considering here, which require the yaw angles (Bragg angles) of all crystals to be fixed. Such multi-crystal error occurs naturally as a result of the cavity alignment procedure. Cavity alignment starts with installation of crystal C_1 as close as possible to 45° to the incident beam; however, this placement can never be exactly 45°. If the first crystal is misaligned by yaw angle δ_1, then the reflected beam is 2δ_1 off the optical axis. To achieve the highest reflectivity at every next crystal, the second, third, and fourth crystals have to be misaligned by angles 3δ_1, 5δ_1, and 7δ_1, respectively, as shown in Fig. 7(d). The beams reflected from these crystals are 4δ_1, 6δ_1, and 8δ_1 off the optical axis, respectively. In this scenario, we assume that no lenses are installed.

In later sections, we study the effects of such crystal alignment errors on x-ray beam dynamics in the cavity; however, we first consider a pure crystal cavity without lenses, in which the effect of the angular and spatial errors can be disentangled.

Other possible misalignment errors discussed later are presented in Fig. 8.

D. Lensless cavity with crystal alignment errors

Figure 9 shows simulation results of x-ray beam dynamics in the four-crystal cavity without lenses with systematically misaligned crystal yaw angles, corre-
FIG. 9: Simulation results of the beam dynamics in the rectangular four-crystal cavity without lenses with systematically misaligned crystal yaw angles.

FIG. 10: Similar to Fig. 9, but with roll angle error $\delta$ in crystal C. The dashed lines show out-of-cavity-plane deflections.

FIG. 11: Similar to Fig. 9, but with roll angle error $\rho$ in crystal C. The dashed lines show out-of-cavity-plane deflections.

FIG. 12: Similar to Fig. 9, but with spatial error $\xi$ in crystal C. Numerical simulation results when crystal C has yaw an-

sponding to Fig. 7(d). Figures 10, 11, and 12 show nu-

merical simulation results when crystal C has yaw an-
gle alignment error $\delta$, roll angle error $\rho$, or spatial alignment error $\xi$, respectively, corresponding to Fig. 7(a)-(c). In all these figures, the results are organized like those for the perfectly aligned cavity in Fig. 6, with one exception: in Figs. 9(i)-(l) and 10(i)-(l), the time response in XBIMs $D_1-D_4$ is shown on a linear scale. Each figure includes data for a perfectly aligned lensless cavity.

The intra-cavity intensity half lifetime increases from 10.6 cycles for a perfect cavity with lenses (Fig. 6) to 12.7 cycles for a perfect lensless cavity, because the lenses and their associated losses are absent.

For all instances of the lensless cavity (including perfectly aligned) the beam size rapidly increases by $\simeq 40 \mu m/cycle$ (rms), because there is no refocusing.

For cavities with yaw angle errors, each cycle increases both the angular and spatial deviation of the beam from the optical axis at both source and midpoint. The angular deviation increases linearly, and the spatial deviation increases quadratically. The systematic multicrystal x-ray beam produces an effect 4 to 5 times larger than the one-crystal yaw angle error. Already after a few cycles, the angular deviations become larger than the half width (4.5 $\mu$rad) of the angular width of the 400 Bragg reflection from diamond. As a result, leakage through the crystals increases, causing increased signals at XBIMs $D_1-D_4$ compared to the perfectly aligned lensless cavity [see Figs. 9(i)-(l) and Figs. 10(i)-(l)]. The intra-cavity intensity also decreases rapidly with yaw angle error $\delta$ [see Fig. 9(g)-(h) and Fig. 10(g)-(h)].

In contrast, the effect of the roll angle error $\rho$ of crystal $C_4$ is much smaller, both on the in-cavity-plane beam position and on the in-cavity-plane angular deviation from the optical axis, as shown by solid lines in Figs 11(a)-(d). The effect is small because there is only a weak coupling between variation in roll angle and variation in the angle of incidence of x-rays to the reflecting atomic planes in the crystals. As a result, the intra-cavity decay curves in Figs. 11(g)-(h) and the signal variations in XBIMs $D_1-D_4$ in Figs. 11(i)-(l) do not differ from those for the perfectly aligned lensless cavity. The main effect of the roll angle error is in the out-of-plane deviation of the beam position and angle at both source and midpoint, as shown by the dashed lines in Figs 11(a)-(d). The roll angle misalignment can be corrected in the lensless cavity by observing the beam profile at the midpoint location.

For all types of crystal angular errors, a positive angular error results in negative angular and negative spatial deviation of the x-ray beam from the optical axis.

The spatial alignment error $\xi$ of crystal $C_4$ results only in a rapid linear increase of the beam position deviation from the optical axis (positive for positive error) at both source and midpoint, while the beam angle does not change. As a result, the decay curves in Figs. 12(g)-(l) are the same as for the perfectly aligned lensless cavity.

In the lensless cavity, the spatial crystal error does not affect the angular beam deviations. This property can be used for cavity alignment, as discussed in Section V.

| Source | Beam position (µm) | Beam angle (nrad) | Beam size (µm) | Half lifetime (cycles) | Oscillation period (cycles) |
|--------|------------------|------------------|----------------|-----------------------|----------------------------|
| Source | 10.82            | 8.67             | 15.17          | 10.8                  | 2.77                       |
| Midpoint | 11.10           | 8.91             | 15.17          | 10.9                  | 2.77                       |

**E. Complete generic cavity with crystal alignment errors**

We now consider a complete four-crystal rectangular cavity with lenses, as in Fig. 1, featuring various crystal alignment errors. Figures 13-16 show numerical simulation results of the x-ray beam dynamics for the following cases: systematically misaligned yaws of crystals $C_1-C_4$ (Fig. 13), one-crystal yaw angle error in $C_4$ (Fig. 14), roll angle error in crystal $C_4$ (Fig. 15), or position error in crystal $C_4$ (Fig. 16). The simulation results in Figs. 13-16 are arranged in the same way as those for the perfect cavity in Fig. 6, with one exception. In panels (a)-(d) of Figs. 13, 14, and 16, we show with thick pink lines the results of calculations using ray-transfer matrices (see Section III B), for comparison with the results obtained with the Shadow3 simulation package [34]. Remarkably, they are practically identical, as long as the angular deviations are much smaller than the angular width of the Bragg reflections.

1. **Betatron oscillations**

Adding the focusing lenses dramatically changes the x-ray beam dynamics in the cavity. For the same crystal alignment errors, the beam size, beam trajectory, and beam monitor response are completely different in the complete cavity.

Unlike the lensless cavity case, any alignment error produces both spatial and angular deflections of the beam from the optical axis.

In all presented cases, the pass-to-pass variations of the spatial or angular deviations from the optical axis as well as of the beam size are much smaller, compared to the lensless cavity analogs shown in Figs. 9-12. The beam size variation and the beam position deflection from the optical axis per cycle are now about 100 times smaller, while the angular deflection per cycle is 10 times smaller, compared to the analogous conditions for the lensless cavity. These changes are clear evidence that the beam size and beam trajectory are stabilized by the lenses. This stabilization takes place only if the parameters and locations of the lenses are chosen properly, as discussed in Section III A. We note that we are considering here the generic cavity case; the confocal cavity case is considered later, in Section IV H.
FIG. 13: Numerical simulation results of x-ray beam dynamics in the rectangular four-crystal generic cavity with systematically misaligned crystal yaw angles.

FIG. 14: Similar to Fig. 13, but with yaw angle error δ in crystal C4.

FIG. 15: Similar to Fig. 14, but with roll angle error ρ in C4. The dashed lines represent out-of-cavity-plane deviations.

FIG. 16: Similar to Fig. 14, but with position error ξ in crystal C4.

Unlike the steadily increasing beam size and increasing spatial and angular beam deviations from the opti-
TABLE IV: X-ray beam characteristics at the source position calculated for various crystal misalignment types from the data in Figs. 13-16. A second sign for offset values is provided if the sign differs between the source and the midpoint. Offset values for both locations are given for the crystal position error case.

| Alignment error | Betatron oscillation type and parameters | Half lifetime (cycles) |
|-----------------|-----------------------------------------|-----------------------|
| Type            | Position (µm) | Angle (nrad) | Size (µm) |                        |
|                 | Offset | Amplitude (rms) | Offset | Amplitude (rms) | Average | Amplitude (rms) |
| None            | 0     | 0.02           | 0     | 0               | 15.47   | 0.26             | 10.8 |
| C₄,C₄ systematic yaw angle δ (nrad) | 50 | 5.41 | 4.03 | 4 | 151 | 15.24 | 0.45 | 10.7 |
|                 | 100   | 10.82          | 8.03  | 9               | 303     | 15.17 | 0.27            | 10.6 |
| C₄ yaw angle δ (nrad) | 200 | 5.49 | 4.69 | ±134 | 188 | 15.25 | 0.33 | 10.6 |
|                 | 400   | 10.99          | 9.34  | ±268            | 375     | 15.24 | 0.39            | 10.4 |
| C₄ roll angle ρ (nrad) | 200 | 3.88 | 3.29 | ±95  | 132 | 15.33 | 0.33 | 10.8 |
|                 | 400   | 7.77           | 6.57  | ±189            | 264     | 15.31 | 0.32            | 10.8 |
| C₄ position ξ (µm) | 10  | 4.81 (-0.09)  | 4.03  | -0.09 (-0.21) | 0.15    | 15.15 | 0.42            | 10.8 |
|                 | 20    | 9.63 (-0.17)  | 8.04  | -0.18 (-0.42)  | 0.29    | 15.34 | 0.41            | 10.7 |

¹ The roll-angle alignment errors result primarily in off-cavity-plane x-ray beam deflections, with the corresponding values shown in the table. The effect on the in-cavity-plane beam deflections is minor and not shown.

d] While simultaneously the offset of the spatial oscillations is non-zero [see Fig. 13(a)-(b)]. A second case is a cavity with position error ξ in crystal C₄ [see Fig. 16(a)], for which the offset of the spatial oscillations does reach zero, but only at the midpoint of the return pass. In all other cases, the oscillation offsets are non-zero, and we will refer to such cases as asymmetric betatron oscillations.

Asymmetric betatron oscillations take place only on one side of the optical axis, with the beam touching or barely crossing the axis. The side on which oscillations occur depends on the sign of the alignment error or on which crystal is misaligned. In the first approximation, the offset of the betatron oscillations is equal to their amplitude. The smallest deflection from the optical axis for any error value or type is near zero (the beam is almost on the optical axis), while the largest deviation equals two amplitudes.

Another common signature can be observed in the beam dynamics in the cavities with angular crystal alignment errors. In all such cases (see Figs. 13-15), the beam characteristics (size and deflections) are very similar, both at the source center and at the midpoint. See, for example, the values in Table III for the case of systematically misaligned yaw angles. Stated another way, the beam monitors at the midpoint reflect the beam status at the source.

This similarity of beam characteristics between source and midpoint is observed in most of the simulations, with one exception. In the case of spatial error in crystal C₄, the offset values of the betatron oscillations at the two locations are different, as shown in Fig. 16. However, the beam size and the amplitudes of the betatron oscillations are much larger than those in Fig. 6, which are due to the artifact arising from use of a finite number of discrete rays in the beam, as discussed in Section IV B. This difference means that the oscillations in Figs. 13-16 are real effects.
oscillations are still the same at both locations.

Table IV presents x-ray beam characteristics at the source location calculated for various crystal misalignment types from the data in Figs. 13-16. Shown are offsets and amplitudes of the betatron oscillations for the beam position, angle, and size. If the offsets have different signs at the two locations, both signs are provided, with the upper sign corresponding to the source center and lower sign to the midpoint location. For the case of position error in crystal $C_4$, we provide offset values for both locations.

The smallest crystal alignment errors shown in the table are chosen such that the rms amplitude of the betatron oscillations for the beam position is less than 5 $\mu$m, i.e., smaller than one third of the 16-$\mu$m rms source size (see Table I). These smallest alignment errors could be considered as alignment error tolerances.

There are several issues to be noted regarding the signs of the offsets. For all positive crystal alignment errors (angular and spatial), the offset of the spatial betatron oscillations is positive at all monitored positions, with one exception, namely, for spatial error at crystal $C_4$. For that case, the spatial betatron oscillations are symmetric with zero offset at the midpoint location. For the angular betatron oscillations, the offset is zero for the systematic misalignment case, negative at both source and midpoint for the case of spatial error in crystal $C_4$, and opposite in sign for the cases of yaw and roll error at crystal $C_4$ (positive offset at the source, negative offset at the midpoint). Note that if a different crystal is faulty, the signs may change relative to those noted in Table IV for errors at crystal $C_4$. For example, a faulty crystal $C_4$ changes the sign of both position and angular oscillation. For a faulty crystal $C_4$, the sign of angular oscillation changes but that of position does not. The reverse is true for a faulty crystal $C_4$, where the position sign changes but the angular sign does not.

The deviations of the beam from the optical axis in the cavity plane are observed to be more sensitive to systematic yaw angle misalignment than to the one-crystal yaw angle misalignment, and least sensitive to roll angle misalignment.

Transverse beam size oscillations observed in panels (e)-(f) of Figs. 13-16 do not change either with the type or magnitude of the alignment errors and have the same origin as those in the perfectly aligned cavity, see Figs. 6(e)-(f) and discussion in Section IV B.

2. Cavity ringdown curves

In contrast to the lensless cavity, the angular beam variations due to the crystal alignment errors are much smaller than the width of the Bragg reflections. As a result, the intra-cavity ringdown curves in panels (g)–(h) of Figs. 13, 14, and 16, together with their half lifetimes, do not change substantially and are close to those of the perfectly aligned cavity case. For the roll angle misalignment case, the ringdown curves practically do not change at all; see Figs. 15(g)-(h). This lack of change is due to weak coupling between the variation of the crystal roll angle and the variation of the angle of incidence of x-rays to the Bragg reflecting atomic planes in the crystals. Similar behavior is observed in the analogous lensless cavity case presented in Fig. 11.

The ringdown curves in panels (j)-(l) of Figs. 13, 14, and 16, reflecting leakage of x-rays through crystals $C_2$-$C_4$, reveal higher sensitivity to crystal errors. The betatron oscillations can be detected by XBIMs $D_2$-$D_4$, as calculations in panels (j)-(l) show. They are practically invisible at XBIM $D_1$ [panel (i) in each figure], reflecting output coupling of x-rays through crystal $C_1$. Additional simulations (not presented here) show that the visibility of the betatron oscillations at XBIM $D_1$ increases with the thickness of crystal $C_1$.

Although crystals $C_2$-$C_4$ have identical thicknesses, the ringdown curves in panels (j)-(l) of Figs. 13, 14, and 16 are different. Additional simulations show that this difference has two causes: first, the asymmetric shape of the Bragg reflection angular dependence, and second, the presence of a dispersive crystal setting. As a result, angular deflection from the Bragg peak always has a different sign from the preceding reflection and, therefore, a slightly different reflectivity.

F. Complete generic cavity with misaligned lenses

In the next step, we consider the complete four-crystal rectangular cavity as in Fig. 1, now including x-ray lenses with angular and spatial alignment errors. Figure 17 shows numerical simulation results of the x-ray beam dynamics in the cavity with lens $L_1$, having yaw angle error $\delta$, while Fig. 18 shows results for lens $L_1$ having lateral position error $\xi$. The simulation results in Figs. 17-18 are organized in the same way as those for the cavity with crystal alignment errors (Figs. 13-16). Table V presents relevant x-ray beam characteristics, organized analogously to Table IV for the crystal error cases.

The x-ray beam dynamics are very insensitive to angular errors at the lens. This behavior is expected because the x-ray beam (a few tens of micrometers in cross-section) is at almost normal incidence to the nearly flat apex of the parabolic surface of the lens (radius of curvature 200 $\mu$m). The angular errors must be in a radian range to produce any significant distortion of x-ray beam trajectory.

In contrast, the lateral spatial errors at the lens are as critical for x-ray beam dynamics as spatial errors at the crystals. The lateral spatial error tolerance is $|\xi| \lesssim 10$ $\mu$m, very similar to the crystal spatial error case (compare Tables IV and V). The ringdown curves also have similar behavior for both crystals and lenses.
TABLE V: X-ray beam characteristics at the source position simulated for the cavity with yaw angle error $\delta$ or lateral spatial error $\xi$ of one lens derived from the data in Figs. 17-18. A second sign for offset values is provided if the sign differs between the source and the midpoint.

| Alignment error | Betatron oscillation type and parameters | Half lifetime (cycles) |
|-----------------|----------------------------------------|-----------------------|
|                 | Position (µm) | Offset | Amplitude (rms) | Angle (nrad) | Offset | Amplitude (rms) | Size (µm) | Average | Amplitude (rms) |
| Type            | Value        |        |                |              |        |                |          |         |                |
| None            | 0            | 0.00   | 0.02           | 0.00         | 0.00   | 0.00           | 15.47    | 0.26    | 10.8            |
| $L_1$ yaw angle $\delta$ (mrad) | 10          | 0.00   | 0.04           | 0.00         | 0.00   | 0.00           | 15.24    | 0.39    | 10.8            |
|                 | 100          | 0.00   | 0.04           | 0.00         | 0.00   | 0.00           | 15.25    | 0.40    | 10.8            |
| $L_1$ position $\xi$ (µm) | 10          | -4.80  | 4.31           | ±123         | 158    | 15.26          | 0.34     | 10.6    | 10.4            |
|                 | 20           | -9.60  | 8.63           | ±246         | 316    | 15.21          | 0.39     | 10.4    | 10.4            |

G. Perfect generic cavity with misaligned x-ray source

Betatron oscillations of the x-ray beam can be induced even in a perfectly aligned cavity, provided the x-ray source is misaligned, as shown in our first analysis of betatron oscillations using analytical methods, in Section III A 2.

The numerical simulations of the beam dynamics for this case are shown in Figs. 19-20, and the beam characteristics are presented in Table VI.

Both the angular and spatial source misalignment types result in symmetric betatron oscillations of the x-ray beam position and angle (see Figs. 19-20, respectively), in agreement with analytical calculations represented by Eq. (18). Both approaches—analytical and numerical—also agree quantitatively. The thick pink lines in Figs. 19-20 show results calculated with the raytransfer matrix approach; they are almost identical to the red lines for the results calculated numerically with the Shadow3 package [34] for the same magnitudes of the alignment errors.

The sensitivity to the source alignment errors is com-
TABLE VI: X-ray beam characteristics at the source position simulated for a cavity with yaw angle alignment error $\delta$ or lateral spatial error $\xi$ at the source as derived from the data in Figs. 19-20.

| Alignment error | Betatron oscillation type and parameters | Half lifetime (cycles) |
|----------------|-----------------------------------------|-----------------------|
|                | Position (µm) | Angle (µrad) | Size (µm) | |
| Type           | Offset (µm) | Amplitude (rms) | Offset (µrad) | Amplitude (rms) | Average (µm) | Amplitude (rms) | |
| None           | 0           | 0.00          | 0.00          | 0.00          | 15.47        | 0.60          | 10.7          |
| Source angle $\delta$ (nrad) | -0.10       | 4.41          | 7             | 178           | 15.30        | 0.51          | 10.7          |
| Source position $\xi$ (µm) | 5            | 3.58          | 3             | 134           | 15.27        | 0.42          | 10.7          |
|                | 10          | 0.3           | 7.17          | 6             | 259          | 15.16        | 0.38          | 10.7          |

parable to the sensitivity to alignment errors of the optical elements. The smallest alignment errors in Table VI can be considered as source alignment tolerance.

H. Misaligned confocal cavity

So far in this section we have used numerical methods to study x-ray beam dynamics in a generic four-crystal rectangular x-ray cavity. Here we address x-ray beam dynamics in a confocal cavity, which we studied partially using analytical methods in Section III A.1. The only difference to the generic cavity case is a different choice of the focal length of both lenses, which is now $f^{(1)} = f/4 = 16.3$ m (see Table I). In the confocal cavity case, Gaussian beams with any Rayleigh length $L_r$ are stable and self-consistent solutions. In our calculations, we will use the same parameters for the Gaussian x-ray source as in the generic cavity case.

Figures 21-24 show numerical simulation results of the x-ray beam dynamics in the confocal cavity with different alignment errors: systematically misaligned yaw angles at crystals $C_i$, $C_j$ (Fig. 21), one-crystal yaw angle error $\delta$ at $C_i$ (Fig. 22), position error $\xi$ at crystal $C_i$ (Fig. 23), and a lateral position error $\eta$ at the source (Fig. 24).
FIG. 21: Numerical simulation results of x-ray beam dynamics in the confocal rectangular four-crystal cavity with systematically misaligned crystal yaw angles.

FIG. 22: Similar to Fig. 21, but with yaw angle error $\delta$ at crystal $C_4$.

FIG. 23: Similar to Fig. 21, but with position error $\xi$ at lens $L_1$ (Fig. 23). The simulation results in Figs. 21-24 are arranged in the same

(Fig. 24), and position error $\xi$ at lens $L_1$ (Fig. 23). The simulation results in Figs. 21-24 are arranged in the same
way as those for the generic cavity in Figs. 13-16.

Just as in the generic cavity, alignment errors in the confocal cavity result in betatron oscillations (both symmetric and asymmetric) of the x-ray beam position and angle. Unlike the generic cavity case, however, the beam size at the monitored locations is stable; there are no beam size oscillations, in agreement with Eq. (8). Also unlike the generic cavity, the beam sizes at the source and the midpoint are different. At the midpoint, the beam size is demagnified to $\approx 9.8 \, \text{µm}$ from $\approx 15.8 \, \text{µm}$ at the source location due to a demagnification factor of $M = 0.62$, in agreement with $M = f^{(1)} / Z_e$ of Eq. (6).

For the same magnitudes of the alignment errors, the magnitudes of the spatial and angular beam displacements from the optical axis are close to those observed in the generic cavity discussed earlier.

However, there are some substantial differences. The period of the betatron oscillation in a confocal cavity is exactly 2 cycles (compare to 2.77 cycles in the generic cavity, in agreement with analytical simulations in Section III A 1 [see Eq. (8)].

Due to this two-cycle period, for all types of alignment errors of the optical elements in a confocal cavity, the x-ray beam returns to the initial position on the optical axis every second pass. The angular beam deviations show similar behavior, but in some cases the angular deviations are always zero, i.e., completely insensitive to some types of alignment errors, such as systematic angular misalignment and spatial error at crystal $C_y$.

This property, however, does not extend to the source alignment errors. From Eq. (8) and results of numerical simulations that are not shown here, the x-ray source error is reproduced every second cycle. The beam size, however, either does not change at the source origin, provided the source errors are involved, or varies insignificantly by $0.15 \, \text{µm}$ (rms) because of the optical elements errors.

These very interesting properties of the confocal cavity can be used to mitigate tolerances on CBXFEL cavity alignment errors (albeit not on the source errors). For this approach to work, however, the electron bunches should arrive with a periodicity matching the betatron oscillations, i.e., with a period equal to two round-trip times of x-rays in the optical cavity. This approach also halves the cavity size for the given electron beam repetition rate, but at a cost of increased cavity losses, as every second round trip is idle.

Ringdown curves in the confocal cavity are of course not identical to those in the generic cavity, showing instead some nuanced differences. However, the decay times are similar.

### V. CAVITY ALIGNMENT

There are tens of degrees of freedom of the optical elements in CBXFEL cavities (close to 30 in the rectangular four-crystal cavity considered in this paper)—many more than in a classical laser oscillator cavity. All these degrees of freedom have to be aligned with a precision ensuring that the to-be-amplified x-ray beam a few tens of microns in cross-section returning into the undulator meets a fresh electron bunch of a similar size.

The effects of different alignment errors are (in most cases) entangled. Where should cavity alignment start, and how should it be performed? The results of the numerical simulation presented in Section IV can be used to propose a strategy for cavity alignment.

First, we recall that in the lensless cavity the spatial crystal error does not affect the angular beam deviations (see Fig. 12). Similarly, the roll angle crystal errors in the lensless cavity produce very small effects on the in-cavity-plane angular beam deviations (see Fig. 11).

As a result, the angular and spatial errors can be decoupled by first aligning crystals in the absence of lenses and then moving in and aligning the lenses. The full procedure would be as follows:

1. With lenses removed, align crystal angles (yaw and roll).
2. Align crystal positions.
3. Move in and align lenses.
4. Adjust the round-trip time to the periodicity of the electron bunches by changing simultaneously the longitudinal positions of two crystals (e.g., $C_x$ and $C_y$) and optimizing the CBXFEL gain.

Time-resolved signals from XBIMs $D_1, D_2, D_3,$ and $D_4$ and from the XBPM at the midpoint are essential for all steps in the alignment.

As noted earlier, the results of our studies show that the XBPM at the midpoint reflects the beam status at the source. This fact is very useful, as in practice it is much easier to monitor the beam at the midpoint than in the undulator.

### VI. DISCUSSION, CONCLUSIONS AND OUTLOOK

We are studying spatial, angular, and temporal behavior of x-ray beams generated by a Gaussian source and stored in a stable x-ray cavity (i.e., x-ray beam dynamics) using analytical methods (paraxial ray-transfer matrix, wave-optics Gaussian beam methods) and numerical ray-tracing computer codes. An example of a rectangular cavity with a 65-m round-trip length is considered, which is designed for a test cavity-based XFEL [23]. The cavity is composed of four Bragg-reflecting flat crystal mirrors located in the corners of the rectangular cavity and two lenses in two symmetry points (see Fig. 1). The focal length of the lenses is chosen to ensure a stable, self-consistent solution for the Gaussian beam in the cavity.

The analytical approaches allow us to determine two stable self-consistent solutions, which we here term the confocal and generic cases. Both cases are studied here.

The analytical approaches are powerful, but they are limited in some respects because the cavity opti-
cal components—the crystals and lenses—are treated in a simplified fashion that neglects photoabsorption and the strongly restricted angular and spectral ranges of Bragg reflections. Because of these limitations, the analytical approach does not provide information about beam intensity that is essential for cavity diagnostics, namely, the intensity of the x-ray beams stored in the cavity, output-coupled from the cavity, or leaked through cavity crystals. The numerical approach removes these limitations. Both approaches, however, provide similar results for the beam position and angle, if the alignment errors are small.

Our studies are focused on the impact on x-ray beam dynamics of spatial and angular alignment errors of the optical components and of the x-ray source.

Most of the alignment errors result in reduced lifetime of x-rays stored in the cavity. But, any misalignment of an optical component or the x-ray source results in periodic betatron-like oscillations of the x-ray orbit in the cavity. The period of the betatron oscillations is a non-integer number (in a general case) of the passes of the stored x-ray beams in the cavity. The period is independent of the type of misalignment and is defined by the parameters of the cavity and x-ray source. The betatron oscillation period is different for the confocal and generic cavities.

The amplitude and offset of the betatron oscillations are signatures of the misalignment type. The betatron oscillations are either symmetric, with zero offset, or asymmetric, with the offset magnitude equal to the amplitude of the oscillations. The amplitude and offset of the betatron oscillations are proportional to the magnitude of the alignment error. The offset sign depends on the sign of the alignment error, on the location of the faulty optical element, and on the monitored location. In general, the presence of betatron oscillations is a signature of cavity misalignment.

In all misalignment cases, the amplitude of the betatron oscillations are practically identical at the source and midpoint locations. The x-ray beam sizes at these locations can differ by a magnification factor. These facts are of practical importance for cavity diagnostics and alignment, as monitoring at the midpoint is easier than in the undulator. However, the offset signs of the betatron oscillations can be different at the source and midpoint locations. In one case considered in the paper, even the magnitude of the offset can differ at the source and midpoint locations. This happens due to the crystal position error (see Fig. 16).

Transverse beam size at the source and midpoint locations is stable independent of the type and magnitude of the alignment errors. Beam size oscillations may appear even in a perfectly aligned cavity if the spatial and angular source parameters are not equal to those of a Gaussian beam with Rayleigh length $Z_r$ at its waist [See Eq. (22) and Table I].

Tolerances of $\simeq 5 - 10 \mu$m in positional alignment and $\simeq 50 - 200$ nrad in yaw angle alignment of the crystal mirrors are required to achieve close to the perfect half lifetime of 10.5 passes of the stored in the cavity x-ray beam power and a betatron oscillation amplitude close to zero. Similar tolerances are required for the lens position errors and for the source angle and position errors.

The angular and spatial x-ray beam dynamics results [see panels (a)-(d) of Figs. 13-20] obtained with numerical simulations are practically identical to those obtained with the ray-transfer matrix approach, as long as the angular deviations are much smaller than the angular width of the Bragg reflections.

For any misalignment type of the optical elements in the confocal cavity, the x-ray beam position returns on the optical axis every second pass. This property may be used to mitigate alignment tolerances for the CBXFEL cavity, provided electron bunches are arriving every second pass of x-rays in the cavity. This approach may also halve the cavity size for the given electron repetition rate, but at a cost of increased cavity losses, because the x-ray pulse is amplified only each second round trip.

Caution is required in using a confocal cavity, as small variations of the cavity parameters may result in beam instabilities. For example, slightly changing the focal length $f = l/4$ to $f(1 + \epsilon)$ ($|\epsilon| \ll 1$) may slightly change the period of the betatron oscillations from exactly 2 to $2 + \delta$ passes, without causing beam instabilities. However, breaking the cavity symmetry by displacing lenses along the optical axis from the symmetry points may result in beam instabilities.

Betatron oscillations and reduced lifetime of x-rays stored in the cavity are also expected to be the typical signatures of misalignments for x-ray cavities of other types. More studies are required, including wavefront propagation simulations, to scrutinize the obtained results and apply them to computer-assisted cavity alignment procedures, including strategies based on machine learning.

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