

WAKE MONOCHROMATOR IN ASYMMETRIC AND SYMMETRIC BRAGG AND LAUE GEOMETRY FOR SELF-SEEDING THE EUROPEAN X-RAY FEL

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Abstract

We discuss the use of self-seeding schemes with wake monochromators to produce TW power, fully coherent pulses for applications at the dedicated bio-imaging beamline at the European X-ray FEL, a concept for an upgrade of the facility beyond the baseline previously proposed by the authors. We exploit the asymmetric and symmetric Bragg and Laue reflections (sigma polarization) in diamond crystal. Optimization of the bio-imaging beamline is performed with extensive start-to-end simulations, which also take into account effects such as the spatio-temporal coupling caused by the wake monochromator. The spatial shift is maximal in the range for small Bragg angles. A geometry with Bragg angles close to $\pi/2$ would be a more advantageous option from this viewpoint, albeit with decrease of the spectral tunability. We show that it will be possible to cover the photon energy range from 3 keV to 13 keV by using four different planes of the same crystal with one rotational degree of freedom. More information and details can be found in [1].

INTRODUCTION

One of the highest priority for experiments at any advanced XFEL facility is to establish a beamline for studying biological objects at the mesoscale, including large macromolecules, macromolecular complexes, and cell organelles. This requires 2-6 keV photon energy range and TW peak-power pulses [2] - [6]. However, higher photon energies (up to 13 keV) are needed to reach the K-edges of commonly used elements, such as Se, for anomalous experimental phasing. Studies at intermediate resolutions need access to the water window at 0.5 keV. The pulse duration should be adjustable from 2 fs to 10 fs.

A basic concept and design of an undulator system for a dedicated bio-imaging beamline at the European XFEL was proposed in [7], and optimized in [8]. All the requirements in terms of photon beam characteristics can be satisfied by the use of a very efficient combination of self-seeding, fresh bunch and undulator tapering techniques [9] - [20]. In particular, a combination of self-seeding and undulator tapering techniques would allow to meet the design TW output power. The bio-imaging beamline would be equipped with two different self-seeding setups. For soft X-ray self-seeding, the monochromator consists of a grating [9]. Starting around the energy of 3 keV it is possible to use a single crystal (wake) monochromator instead of a grating [8].

In [8] we demonstrated that it will be possible to cover the photon energy range between 3 keV and 13 keV using the C(111), C(220) and C(004) symmetric Bragg reflections. In this scenario, three different crystals would enable self-seeding for the different spectral range. In particular, we proposed to exploit the C(111) symmetric Bragg reflection in the photon energy range between 3 keV and 5 keV.

While developing a design for the bio-imaging beamline, the authors first priority was to have it satisfying all requirements. Having achieved that goal, the next step is to optimize the design, making it as simple as possible. The design presented here aims for experimental simplification and cost reduction of the self-seeding setups. In order to improve the original design, here we propose to exploit asymmetric Bragg and Laue C(111), C(113) and C(333) reflections together with the symmetric Bragg reflection C(004). The novel design of the self-seeding setup combines a wide photon energy range with a much needed experimental simplicity. Only one diamond crystal is needed, and only one rotational degree of freedom is required.

While, in this article, we consider applications for the bio-imaging beamline in particular, the present study can also be applied to other beamlines, for example the SASE1-SASE2 lines at the European XFEL as well.

DYNAMICAL DIFFRACTION THEORY AND ASYMMETRIC-CUT CRYSTALS

We begin our analysis of asymmetric-cut crystals by specifying the scattering geometry under study. With reference to Fig. 1, and following the notation in [21] we identify the crystal surface with the unit vector normal to the crystal surface \vec{n} , directed inside the crystal. The unit vector \vec{s} indicates the trace of the Bragg planes. The direction of the incident beam is specified by the unit vector \vec{s}_0 , while that of the diffracted beam is given by \vec{s}_h . Always following [21], we call ψ_n the angle between \vec{n} and \vec{s} , ψ_0 the angle between \vec{n} and \vec{s}_0 , and ψ_h the angle between \vec{n} and \vec{s}_h . The signs of these angles are univocally fixed by requiring that the angle between \vec{s} and \vec{s}_0 is positive (and equal to the Bragg angle θ_B), while the angle between \vec{s} and \vec{s}_h is negative (and equal to $-\theta_B$). Figure 1 shows two generic examples for both Bragg and Laue geometries.

Let us consider an electromagnetic plane wave in the X-ray frequency range incident on an infinite, perfect crystal. Within the kinematical approximation, according to the Bragg law, constructive interference of waves scattered

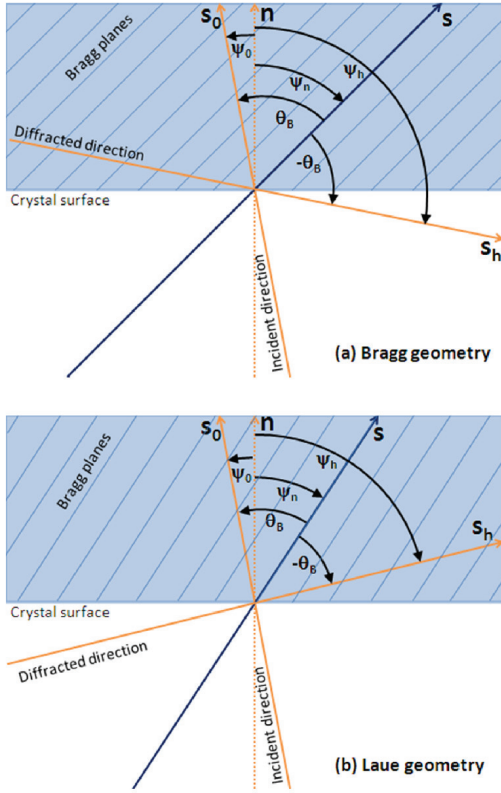


Figure 1: Sketch of (a) Bragg and (b) Laue scattering geometry.

from the crystal occurs if the angles between the reflecting lattice planes and both incident and reflected beams are equal to Bragg angle θ_B (Fig. 1). The wavelength λ and the Bragg angle are related by the well known equation

$$\lambda = 2d \sin(\theta_B), \quad (1)$$

where d is the distance between Bragg planes, and from now on we assume reflection into the first order. This equation shows that for a given wavelength of the x-ray beam diffraction is possible only at certain angles determined by d . It is important to remember the following geometrical relationships:

- In the kinematical approximation, the Bragg reflection is a mirror reflection i.e. the angle between the incident X-ray beam and the normal to the Bragg planes is equal to that between the normal and the reflected beam.
- The incident beam and the forward diffracted (i.e. the transmitted) beam have the same direction.

Diffraction from an asymmetric-cut crystal is equivalent to diffraction from a blazed grating. This equivalence has already been noted in [22]. The Bragg-reflected light from an asymmetric-cut crystal behaves as the light diffracted from a grating with period $D = d / \cos(\psi_n)$ and is dispersed in accordance with the grating equation

$$\lambda = D[\sin(\psi_0) - \sin(\psi_h)]. \quad (2)$$

When the Bragg condition Eq. (1) and the mirror reflection condition are simultaneously met one obtains

$$\psi_0 = \psi_n + \theta_B \quad (3)$$

and

$$\psi_h = \psi_n - \theta_B \quad (4)$$

By direct substitution in Eq. (2) and using simple trigonometric relations, it is easy to check that Eq. (3) and Eq. (4) satisfy the grating equation.

We now turn our attention beyond the kinematical approximation to the dynamical theory of diffraction by a crystal. With reference to Fig. 1, let us define the angle between the crystal surface and the input beam as $\theta_i = \pi/2 - \psi_0$. Similarly, we define the diffracted angle $\theta_d = \pi/2 - \psi_h$, with θ_d a function of the frequency, according to Eq. (2). We also define the angle between the Bragg planes and the crystal surface as $\alpha = \pi/2 - \psi_n$. All these new quantities follow the previously defined convention as concerns their signs. Note that Eq. (3) and Eq. (4) can be rewritten in terms of incident and diffracted angles as $\theta_d = \alpha - \theta_B$ and $\theta_i = \alpha + \theta_B$.

It is useful to describe the modification of the incident beam by means of a transfer function. The reflectivity curve - the reflectance - can be expressed in the frame of dynamical theory as

$$R(\theta_i, \theta_d, \omega) = R[\Delta\omega + \omega_B \Delta\theta_i \cot(\theta_B), \Delta\theta_d], \quad (5)$$

where $\Delta\omega = (\omega - \omega_B)$, $\Delta\theta_i$, and $\Delta\theta_d$ are, respectively, the deviations of frequency, incident angle and diffracted (i.e. reflected) angle from the resonance (Bragg) frequency and angles, respectively. The frequency ω_B and the angle θ_B are given by the Bragg law $\omega_B \sin(\theta_B) = \pi c/d$.

Consider now a perfectly collimated, white beam incident on the crystal. Within the kinematic approximation, the transfer function as a function of the first argument is a Dirac δ -function, $\delta[\Delta\omega + \omega_B \Delta\theta_i \cot(\theta_B)]$ which is another representation of the Bragg law in differential form:

$$\frac{d\lambda}{d\theta_i} = \lambda \cot(\theta_B). \quad (6)$$

In addition to this, within the kinematic approximation, reflection from a lattice plane is always a mirror reflection, and

$$\frac{d\theta_d}{d\theta_i} = 1. \quad (7)$$

Moving to the framework of the dynamical theory, and in contrast to what has just been said, the reflectivity width is finite. This means that there is a reflected beam even when the incident angle and the wavelength of the incoming beam are not exactly related by the Bragg equation. It is interesting to note that incident beam and transmitted beam continue to have the same direction also in the framework of dynamical theory. However, in the framework of the dynamical theory and in the case of asymmetric-cut crystal, the reflection from lattice planes are not a mirror reflection anymore: the grating equation Eq. (2), holds, and the reflection from the crystal surface is always a grating reflection.

The diffraction from the asymmetric-cut crystal in Bragg and Laue geometry can be described an asymmetry parameter, b , defined by

$$b = \frac{\vec{n} \cdot \vec{s}_0}{\vec{n} \cdot \vec{s}_h} = \frac{\cos(\psi_0)}{\cos(\psi_h)}. \quad (8)$$

In literature on X-ray crystal diffraction, the asymmetry parameter is sometimes defined as inverse of b , and indicated with the letter γ , for example in [21]. Here we follow the same convention used in [22]. Note that $|b| = \sigma_{\text{in}}/\sigma_{\text{out}}$ is the ratio of the widths of incident and diffracted beams. From Eq. (2) follows that

$$b = \frac{d\theta_d}{d\theta_i}. \quad (9)$$

As has been pointed out elsewhere, this is a consequence of Liouville theorem [22]. In fact, a quasi-monochromatic, collimated beam of finite width that is reduced in width must be dispersed in angle to preserve the space-angle phase volume.

For the Bragg geometry, where the diffracted light exists on the same side of the surface as the incident beam, we have $b < 0$, whereas $b > 0$ describes Laue geometry. In particular, $b = -1$ corresponds the symmetric Bragg diffraction, and $b = 1$ corresponds to the symmetric Laue diffraction.

The dispersion of the diffracted light from the asymmetric-cut crystal follows directly from the grating equation, yielding

$$\lambda \frac{d\theta_d}{d\lambda} = (1 + b) \tan(\theta_B). \quad (10)$$

As expected, there is no dispersion for symmetric Bragg geometry ($b = -1$) because there is no grating structure in that case.

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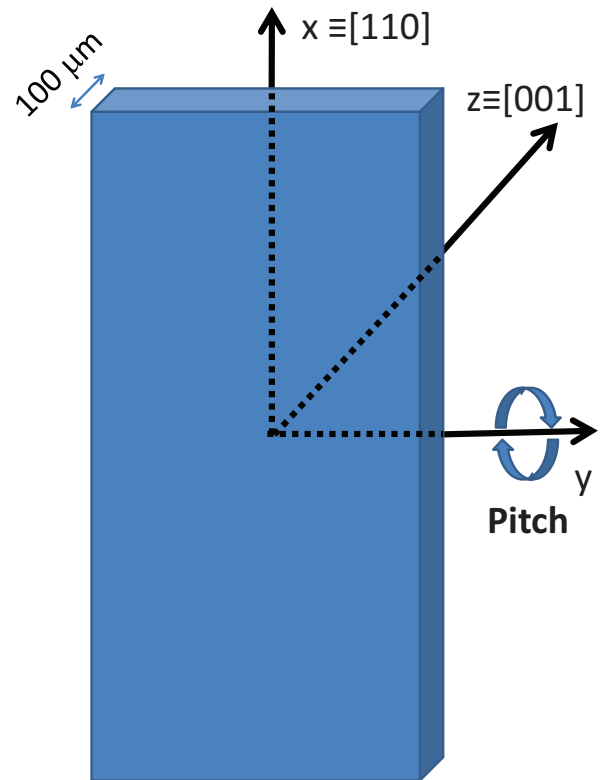


Figure 2: Drawing of the orientation of the diamond crystal considered in this article.

Table 1: Useful Diamond Reflections

| hkl | Min. Energy (keV) | ΔE (meV) |
|-----|-------------------|------------------|
| 111 | 3.01034 | 192.0 |
| 311 | 5.76401 | 56.0 |
| 400 | 6.95161 | 60.6 |
| 333 | 9.03035 | 27.3 |
| 444 | 12.0404 | 25.0 |

In the following, we will consider one single diamond crystal, as the 100 μm thick crystal proposed in [15], and currently used into the LCLS self-seeding setup [23]. We will define a cartesian reference system $\{x, y, z\}$ linked with the crystal. The direction z corresponds to the direction identified by the Miller indexes 0, 0, 1, which also coincides with the direction of \vec{n} , while x and y are specified as in Fig. 2, so that the direction [110] corresponds to the x direction.

The crystal can rotate freely around the y axis (pitch angle) as indicated in the figure. In this way, we can exploit several symmetric and asymmetric reflection: we will be able to cover the entire energy range between 3 keV and 13 keV by changing the pitch angle of the crystal in Fig. 2. In the low energy range between 3 keV and 5 keV we will use the C(111) asymmetric reflection (in Bragg or Laue geom-

etry, depending on the energy). At higher energies between 5 keV and 7 keV we propose to go to the C(113) asymmetric reflection in Bragg geometry. In the range between 7 keV and 9 keV we can use instead the C(004) symmetric reflection, in Bragg geometry. Finally, for energies larger than 9 keV we propose the use of the C(333) asymmetric reflection, in Bragg geometry¹. The list of reflections considered in this article is summarized in Table 1, extracted from [24].

For self-seeding implementation, we are interested in the forward diffracted, i.e. in the transmitted beam for each of these reflections. From this viewpoint, the crystal can be characterized as a filter with given complex transmissivity. We will now consider the three transmissivity separately, showing their amplitude and phase, together with the crystal geometry for fixed energy points.

In Fig. 3 we show the amplitude and the phase for the C(111) asymmetric Bragg reflection at 3.5 keV. The following Fig. 4 shows the same reflection at a higher energy, 5 keV. In this case, one has Laue geometry. In Fig. 5 we plot the same quantities for the C(113) asymmetric Bragg geometry at 7 keV. In Fig. 6 we consider the symmetric Bragg reflection C(004) at 8 keV and, finally, in Fig. 7 we plot amplitude and phase for the asymmetric Bragg reflection C(333) at 9 keV. By inspecting the plots, the reader can easily see the difference between Bragg and Laue geometry, as well as that between symmetric and asymmetric reflections.

As shown in [1], amplitude and phase in the plots are related by Kramers-Kronig relations. The simplest check of the correctness of the calculations by means of dynamical theory consists, therefore, in verifying that amplitude and phase of the transmissivity are actually related by Kramers-Kronig relations.

SPATIOTEMPORAL SHIFT AND ITS INFLUENCE ON INPUT COUPLING FACTOR

A wake monochromator introduces spatiotemporal deformations of the seeded X-ray pulse, which can be problematic for seeding. The spatiotemporal coupling in the electric field relevant to self-seeding schemes with crystal monochromators has been analyzed in the framework of classical dynamical theory of X-ray diffraction [24].

This analysis shows that a crystal in Bragg or Laue geometry transforms the incident electric field $E(x, t)$ in the $\{x, t\}$ domain into $E(x - at, t)$, where $a = \text{const.}$ The physical meaning of this distortion is that the beam spot size is independent of time, but the beam central position changes as the pulse evolves in time. As shown in [1, 25],

¹It should be remarked that above 12 keV the C(444) asymmetric Bragg reflection turns out to be a valid alternative, though results are not explicitly analyzed in this article. The Bragg angle is, in this case, very near to $\pi/2$, $\theta_B = 84.4$ deg, while $\psi_n = 35.3$ deg. The relative Darwin width amount to about $2 \cdot 10^{-6}$, with a very high transmissivity (about 97%). Our calculations show that one can reach pulse power in excess of 600 GW at 12 keV with a FWHM relative bandwidth of about $5 \cdot 10^{-5}$.

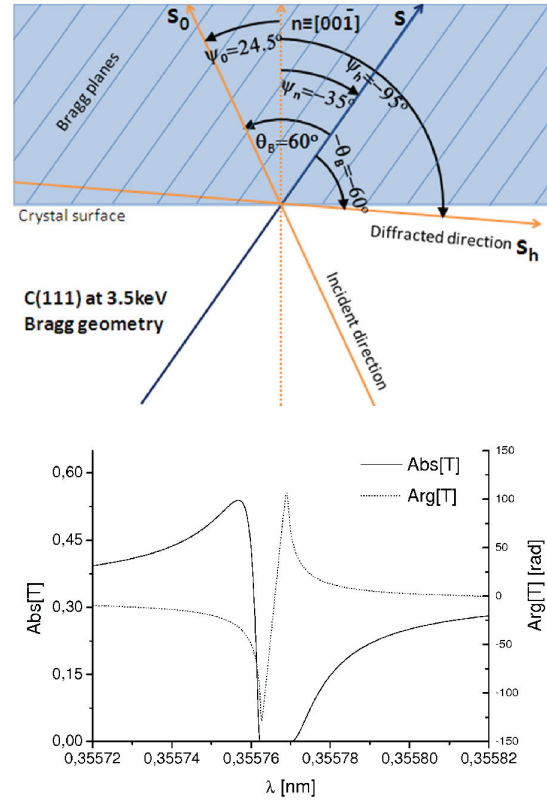


Figure 3: Scattering geometry, modulus and phase of the transmittance for the C(111) asymmetric Bragg reflection from the 100 μm thick perfect diamond crystal in Fig. 2 at 3.5 keV.

based on the only use of the Bragg law, we can directly arrive to an explanation of spatiotemporal coupling phenomena in the dynamical theory of diffraction. In the self-seeding case, where the incoming XFEL beam is well collimated, its angular spread is a few times smaller than the angular width of the transfer function. Yet, the spectral bandwidth of the incoming beam is much wider than the bandwidth of the transfer function. Under the limit of a wide spectral bandwidth for the incoming beam (with respect to the bandwidth of the transfer function), we obtain the following expression for the electric field after the crystal, $E_{\text{out}}(x, t)$:

$$E_{\text{out}}(x, t) = \eta(t) \int dk_x \exp(i \cot \theta_B k_x c t) \times \exp(-i k_x x) E(\omega_B, k_x) = \eta(t) a(x - c \cot \theta_B t), \quad (11)$$

where

$$\eta(t) = \frac{1}{2\pi} \int d\omega \exp(-i\omega t) T(\omega) \quad (12)$$

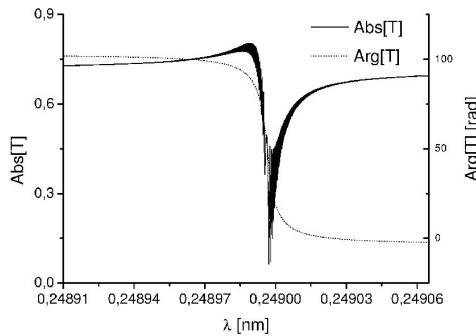
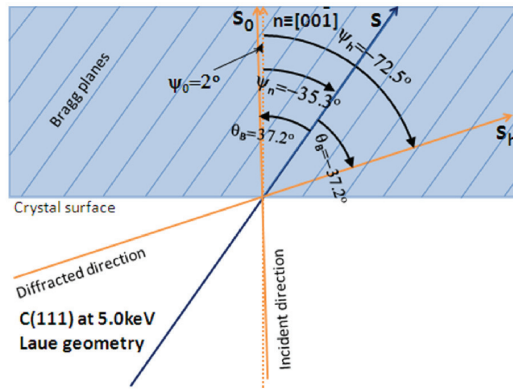


Figure 4: Scattering geometry, modulus and phase of the transmittance for the asymmetric C(111) Laue reflection from the 100 μm thick perfect diamond crystal in Fig. 2 at 5 keV.

is the inverse temporal Fourier transform of the transmittance curve T (i.e. the impulse response of the crystal). Eq. (11) is universal i.e. valid for both symmetric and asymmetric Bragg and Laue geometries.

The spatial shift given by Eq. (11) is proportional to $\cot(\theta_B)$, and is maximal in the range for small values of θ_B . Therefore, the spatiotemporal coupling is an issue, and efforts are necessarily required to avoid distortions. A geometry with θ_B close to $\pi/2$ would be a more advantageous option from this view point, albeit with decrease in the spectral tunability [24].

Influence of the Offset on the Coupling Factor

The influence of the spatiotemporal distortion on the operation of the self-seeding setup can be quantified by studying the input coupling factor between the seed beam and the ground eigenmode of the FEL amplifier. When the undulator is sufficiently long, the output energy in the FEL pulse grows exponentially with the undulator length, and the energy gain, $G = E_{\text{out}}/E_{\text{ext}}$, can be written as

$$G = A \exp[z/L_g], \quad (13)$$

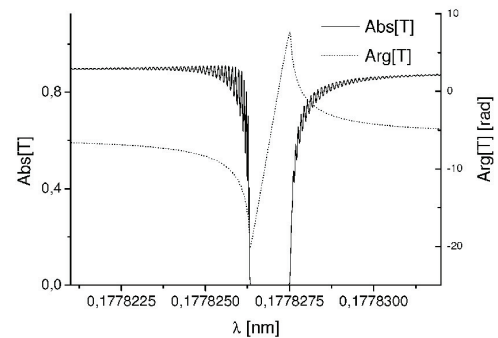
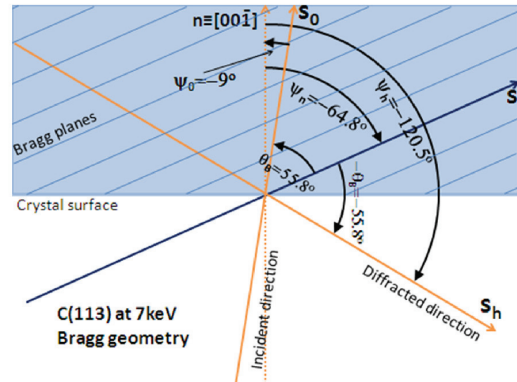


Figure 5: Scattering geometry, modulus and phase of the transmittance for the asymmetric C(113) Bragg reflection from the 100 μm thick perfect diamond crystal in Fig. 2 at 7 keV.

where A is the input coupling factor. In the linear regime the energy gain does not depend on the input energy E_{ext} , and for the case including spatial shift the input coupling factor A allows for a simple and convenient measure of the departure from the ideal situation. In our case this measure is simply defined as

$$Q \equiv \frac{E_{\text{nonideal}}}{E_{\text{ideal}}} = \frac{A_{\text{nonideal}}}{A_{\text{ideal}}}. \quad (14)$$

We will consider a particular example for $\lambda = 0.15$ nm, corresponding to about 8 keV. We simulated the SASE process in the first 11 cells, followed by the self-seeding setup exploiting the C(004) reflection. The seed beam is then superimposed again onto the electron bunch (the modulation having been washed out by the chicane). We calculate the output power and spectrum after 6 cells, which is still in the linear regime, and we scan over the transverse offset.

A few examples of the output obtained with this procedure are shown in Fig. 8, which compares the result for zero offset (black solid lines) with those for 2 μm , 18 μm , and 34 μm (red dotted lines). All results refer to a single simulation shot. The plots on the left show the transverse

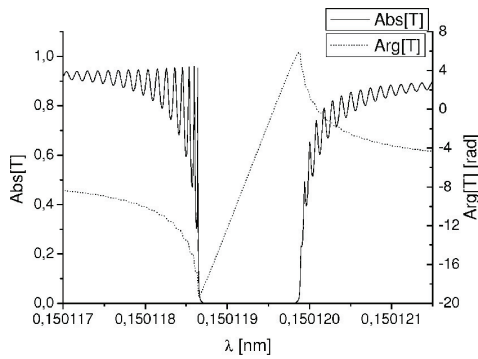
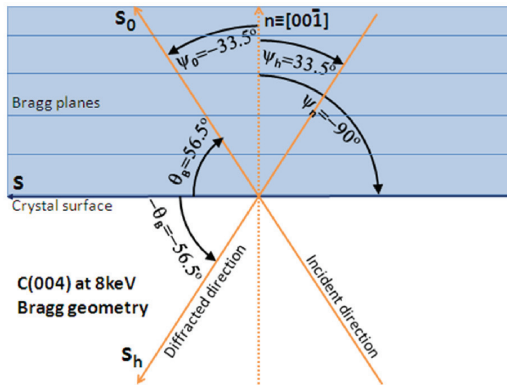


Figure 6: Scattering geometry, modulus and phase of the transmittance for the symmetric C(004) Bragg reflection from the 100 μm thick perfect diamond crystal in Fig. 2 at 8 keV.

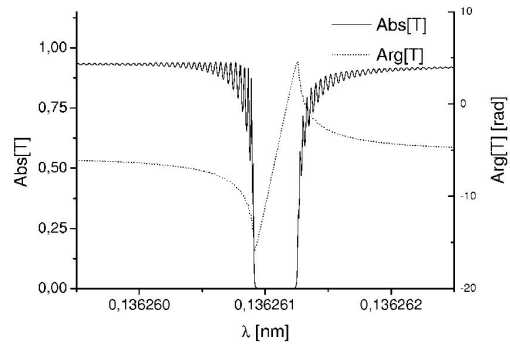
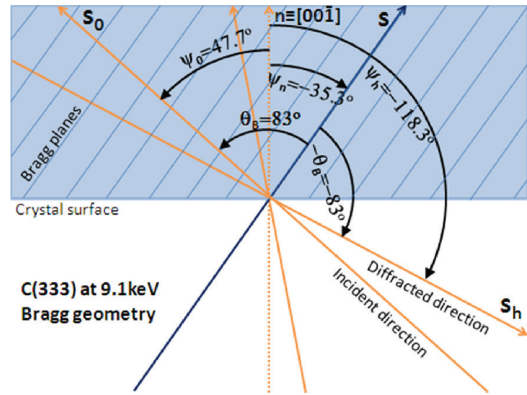


Figure 7: Scattering geometry, modulus and phase of the transmittance for the asymmetric C(333) Bragg reflection from the 100 μm thick perfect diamond crystal in Fig. 2 at 9 keV.

profile of the photon beam after 6 undulator cells following the self-seeding setup. The figures in the middle show the power, and those on the left the spectra. Qualitatively, the effect due to the transverse offset is easy to see by inspection.

The energy as a function of the position into the radiator is shown in Fig. 9. The function $Q(\Delta)$ instead, is shown in Fig. 10. Note that the input coupling factor does not drop abruptly to zero when Δ is of order of the rms transverse size of the photon beam. This is because the photon beam intensity does not drop off as a Gaussian function. As a result, one can qualitatively go to larger deviations of θ_B , still obtaining a reasonable coupling factor.

We hope that these considerations will be useful for FEL physicists in the design stage of wake monochromator setups.

FEL STUDIES

In order to quantitatively investigate the effects of the spatial shift on the FEL amplification process, we performed numerical simulations using the code Genesis [26]. Simulations are based on a statistical analysis consisting

of 100 runs. We consider the setup in Fig. 11, with reference to [8] for details. In this article we are interested in the energy range where hard X-ray self seeding can be implemented, starting from 3.5 keV up to 13 keV. The C(111) reflections (Bragg and Laue) will be used in the second chicane. C(113), C(004) and C(333) reflections will be used in the third chicane. Since we are interested in energies starting from 3.5 keV, we fix the electron energy at 17.5 GeV. The lower energy is used in the very soft X-ray regime, see [8], between 0.3 keV and 0.5 keV, which is outside the interests of this article, and where one relies on a grating monochromator. We used the results of start-to-end simulations [27], while the main undulator parameters are reported in Table 2. Our simulations automatically included the influence of the spatial shift of the photon beam induced by the crystal.

As is explained in detail in [8], in the range between 3 keV and 5 keV the first chicane is not used and is switched off. After the first 7 cells the electron and the photon beams are separated with the help of the second magnetic chicane, and the C(111) reflection is used to monochromatize the radiation. The seed is amplified in the next 4 cells. After

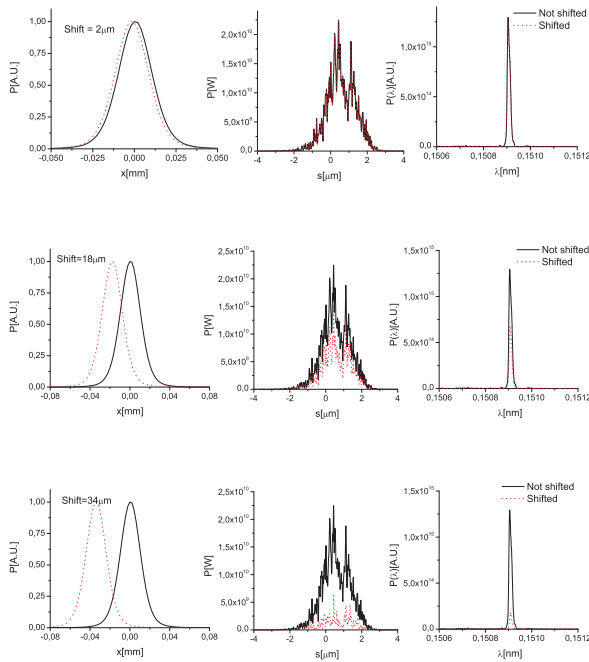


Figure 8: Comparison between the self-seeded output with (red, dotted lines) and without (black, solid lines) transverse offset, at different offset values. The left plots show the photon beam transverse profiles, the middle plots show the power, the right plots show the spectra. All plots refer to a single simulation shot.

Table 2: Undulator Parameters

| Parameter | Units | Value |
|-----------------------|-------|--------|
| Undulator period | mm | 68 |
| Periods per cell | - | 73 |
| Total number of cells | - | 40 |
| Intersection length | m | 1.1 |
| Photon energy | keV | 0.3-13 |

that, the electron and the photon beam are separated again by the third chicane, and an X-ray optical delay line allows for the introduction of a tunable delay of the photon beam with respect to the electron beam. The following 6 cells use only a part of the electron beam as a lasing medium. A magnetic chicane follows, which shifts the unspoiled part of the electron bunch on top of the of the photon beam. In this way, a fresh bunch technique can be implemented. Since the delays are tunable, the photon pulse length can be tuned. Finally, radiation is amplified into the last 23 tapered cells to provide pulses with about 2 TW power.

In partial difference with respect to what has been discussed in [8], for energies lower than 5 keV we used the asymmetric C(111) reflection (Bragg and Laue geometry), while in [8] we exploited the C(111) symmetric Bragg reflection only. Moreover, for energies larger than 5 keV we

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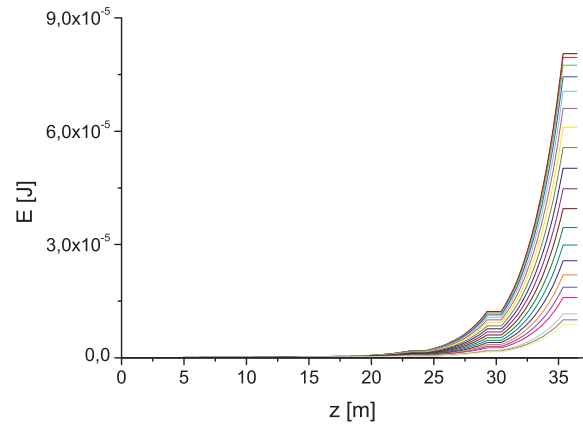


Figure 9: Collected energies as a function of the position inside the radiator, for increasing offset from 0 μm to 40 μm with steps of 2 μm .

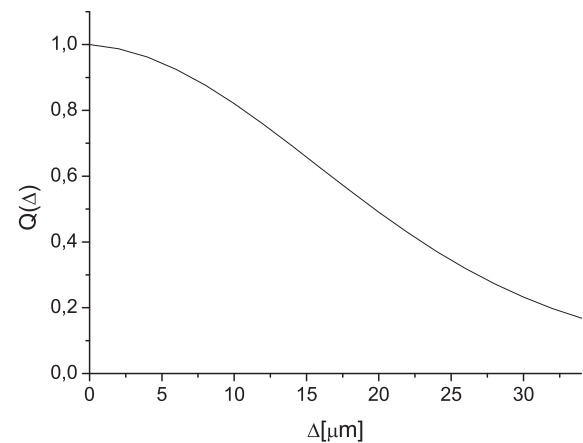


Figure 10: Measure of the dependence of the input coupling factor on the offset $Q(\Delta)$.

rely on a crystal placed after 11 cells, and we take advantage of the C(113), the C(004) and the C(333) reflections. In this case the fourth chicane is switched off. If tunability of the pulse duration is requested in this energy range, this is most easily achieved by providing additional delay with the fourth magnetic chicane installed behind the hard X-ray self-seeding setup.

Results for the different reflections at given energy points were presented in [1]. We concluded that TW-level pulses can be achieved with the help of tapering for energies larger than about 3 keV, spanning over the entire energy range up to about 13 keV.

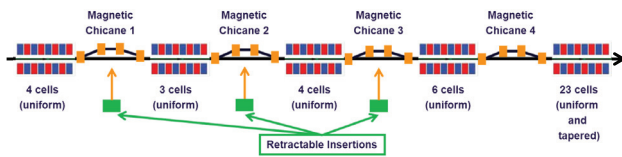


Figure 11: Schematic setup of the bio-imaging beamline discussed in [8].

CONCLUSIONS

Self-seeding scheme with wake monochromators are routinely used in generation of narrow bandwidth X-ray pulses at LCLS [23]. Recently, the photon energy range of self-seeding setup at LCLS was extended from 8 keV to lower photon energies down to 5.5 keV by exploiting different planes on the same diamond crystal [28].

In this article we propose a study of the performance of self-seeding setups for the European XFEL based on wake monochromators, exploiting different (symmetric and asymmetric, Bragg and Laue) reflections of a single diamond crystal, similar to that used into the LCLS setup. In our study we account the spatiotemporal shift of the seed induced by the passage through the crystal, and we study the dependence of the FEL input coupling factor on this shift. We exemplify our results using the concept for a dedicated bio-imaging beamline previously proposed by the authors. We conclude that crystals similar to the one actually used at the LCLS can be exploited to cover the energy range between 3 keV and 13 keV with high performance, allowing one to reach TW-class pulses.

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