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Focusing femtosecond X-ray free-electron laser pulses by refractive lenses

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The possibility of using a parabolic refractive lens with initial X-ray free-electron laser (XFEL) pulses, *i.e.* without a monochromator, is analysed. It is assumed that the measurement time is longer than 0.3 fs, which is the time duration of a coherent pulse (spike). In this case one has to calculate the propagation of a monochromatic wave and then perform an integration of the intensity over the radiation spectrum. Here a general algorithm for calculating the propagation of time-dependent radiation in free space and through various objects is presented. Analytical formulae are derived describing the properties of the monochromatic beam focused by a system of one and two lenses. Computer simulations show that the European XFEL pulses can be focused with maximal efficiency, *i.e.* as for a monochromatic wave. This occurs even for nanofocusing lenses.

Keywords: X-ray focusing; refractive lenses; X-ray free-electron laser; semi-analytical theory; femtosecond pulses.

1. Introduction

The X-ray free-electron laser (XFEL) is now a reality in the USA (LCLS, 2011). Two other projects are under construction, in Japan (SCSS, 2011) and Germany (EXFEL, 2011). In the case of pulse generation in the self-amplified spontaneous-emission (SASE) regime, the European XFEL will produce very intensive pulse trains of duration 100 fs with 10^{12} photons per pulse. In addition, the pulses will be almost fully transverse coherent (TDR, 2007). The pulse train consists of many single spikes of duration 0.3 fs. Various spikes are incoherent; therefore the coherent time is of the same time scale. Such a short duration of pulses corresponds to the energy band ΔE with a base photon energy $E = \hbar\omega$, which is equal to 12.4 keV for the SASE1 beam of the European XFEL. According to the project the relative energy band will be $\Delta E/E \simeq 10^{-3}$.

The new possibility of generating very intensive femtosecond pulses stimulated several theoretical studies on time-dependent X-ray diffraction in single crystals [see Bushuev (2008) and references therein]. As a rule, the response of a perfect crystal to an instantaneous plane incident wave was calculated (Shastri *et al.*, 2001) and then the diffraction of an X-ray wave of arbitrary time structure was taken into account by means of convolution. We note that the crystal diffraction process is ruled by a single parameter, namely the deviation from the Bragg condition, which depends linearly on both the angular shift and the energy shift. It is easy to understand that the response of a perfect crystal to an instantaneous plane incident wave is mathematically completely the same as for the case of a monochromatic spherical wave from a source placed on the entrance surface of the crystal. However, the latter was solved much earlier (Kato, 1961*a*,*b*; Afanasev & Kohn, 1971) in an analytical form. Of course, it is of interest to study the possibilities of using all optical elements with the new XFEL source. Periodical multilayers were considered by Ksenzov *et al.* (2008).

In this article we analyze the possibility of using a parabolic refractive lens (Lengeler *et al.*, 1999) with initial XFEL beams, *i.e.* without a monochromator. It is known that the refractive lens is a dispersive optical element because the refractive index of matter depends on the photon energy. However, this dependence is not strong. The transformation of the pulse time structure by optical elements in this case is not an actual problem because the coherent pulses (spikes) have a time duration of 0.3 fs whereas the full time of the XFEL pulse is 100 fs. The full pulse consists of many spikes, and different spikes are incoherent. Such a situation is similar to the case of a synchrotron radiation pulse from a bending magnet and an undulator pulse, and there is only a quantitative, not a qualitative, difference.

The time duration of a coherent pulse can be estimated from the radiation energy spectrum according to the time–energy uncertainty principle $\Delta t \Delta E \simeq h$, where h is Planck's constant. Correspondingly, the shortest coherent pulses arise in synchrotron radiation from a bending magnet. However, these pulses cannot be measured because it is impossible to select one coherent pulse from the many others which propagate simultaneously. A real synchrotron radiation pulse is determined by the time of flight of a bunch near the window, but this full pulse is incoherent in time and is rather long. Only if the scattering process can make the time structure of the outgoing coherent pulse longer than the full incoherent pulse can this be measured. Such a situation takes place with nuclear resonant (Mössbauer) scattering (Kagan *et al.*, 1979).

Similarly, in the case of XFEL radiation the scattering process has to make a pulse longer than 100 fs in order to be measured. This is impossible with refractive optics as well as with crystals and other optical elements. Therefore, it is sufficient to calculate the integrated intensity over the time duration of a coherent pulse. Using the Parseval formula, this intensity is equal to the intensity of a monochromatic wave integrated over the spectrum of incident radiation. The standard theory of focusing deals only with the space dependence of the monochromatic wave. It is known that focusing is impossible for a white synchrotron radiation beam and that a monochromator is necessary. As follows from our computer simulation, the European XFEL pulses can be focused as well as for the monochromatic wave. Only a small widening of the focused beam can occur in an undulator where $\Delta E/E$ is of the order of 10^{-2}. The excellent focusing occurs even for nanofocusing lenses. Therefore a monochromator is not necessary. This conclusion differs from the conclusion of TDR (2007).

The article is organized as follows. In §2 we derive general formulae in terms of the frequency integral for the two following processes: propagation of short coherent pulses of XFEL radiation in free space, and transmission of such pulses through various objects. Then we consider the one-dimensional case and derive the analytical recurrent relations which allow one to calculate any focusing system consisting of many lenses. In §3 the structure of the incident wave and general properties of the Gaussian wave are discussed. Then the recurrent relations are applied to the cases of one and two lenses, and analytical formulae are derived for the first time. The results of computer simulations for polychromatic radiation are presented in the final section.

2. General approach

As is known, the XFEL beam has a small transverse size, and it propagates over a large distance along a straight line. The diffraction theory of X-ray focusing and imaging with a refractive lens describes two different phenomena. The first one is the propagation of an X-ray wave in a vacuum, and the second one is the transmission of an X-ray wave through objects of various structure. We consider these phenomena separately. The existing theory of focusing describes a monochromatic wave. It is convenient to describe the propagation of a pulse of short time duration in terms of monochromatic theory through Fourier transformation. This allows computer simulations developed for a monochromatic wave to be used.

2.1. Propagation of an XFEL coherent wave in a vacuum

We choose the direction of wave propagation as the optical axis which coincides with the z axis of our coordinate system. Let us suppose that the electric field amplitude $E(x, y, z_0, t)$ is known in some plane normal to the optical axis and located at a distance z_0 from the origin. Here x and y are coordinates inside the plane (see Fig. 1) and t is the time. We do not specify the polarization of the field because it will be the same in all processes under consideration. We will find the relation which describes the transformation of the field during a propagation along the optical axis through free space. The field (wavefunction) in the new plane located at a distance $z_1 = z_0 + z_\mathrm{p}$ is a solution of the Maxwell wave equation in free space,

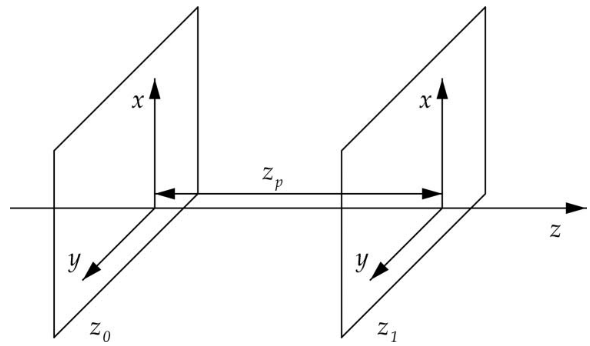

Figure 1
Two planes across the optical axis which coincides with the z-axis of the coordinate system.

$$\left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) E(\mathbf{r}, t) = 0, \qquad \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}, \qquad (1)$$

with the boundary condition at the plane $z = z_0$. Here c is the speed of light, and $\mathbf{r} = x, y, z$. We will find a solution as the Fourier integral

$$E(x, y, z_1, t) = \int \frac{\mathrm{d}\omega\,\mathrm{d}k_1\,\mathrm{d}k_2}{(2\pi)^3}\, E(k_1, k_2, z_0, \omega) \times \exp(-i\omega t + ik_1 x + ik_2 y + ik_3 z_\mathrm{p}), \qquad (2)$$

where

$$E(k_1, k_2, z_0, \omega) = \int \mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y\, E(x, y, z_0, t) \times \exp(i\omega t - ik_1 x - ik_2 y). \qquad (3)$$

Expression (2) has one free parameter, k_3, and coincides with the boundary condition at $z_\mathrm{p} = 0$.

Substituting (2) into (1) we find the free parameter

$$k_3 = \left(\frac{\omega^2}{c^2} - k_1^2 - k_2^2\right)^{1/2}. \qquad (4)$$

We take into account that for XFEL radiation the function $E(k_1, k_2, z_0, \omega)$, as a function of ω, is localized around a very large frequency ω_0 which corresponds to a photon energy $\hbar\omega_0$ of about 12 keV. On the other hand, possible values of k_1 and k_2 are rather small compared with ω_0/c. Therefore we can apply a paraxial approximation with very good accuracy,

$$k_3 = \frac{\omega}{c} - \frac{c}{2\omega}(k_1^2 + k_2^2). \qquad (5)$$

Taking this into account we obtain finally

$$E(\mathbf{r}, t) = \int \frac{d\omega}{2\pi} \exp(-i\omega t)\, E(\mathbf{r}, \omega), \tag{6}$$

where

$$E(x, y, z_1, \omega) = \exp(i\omega z_p/c) \int dx'\, dy'\, E(x', y', z_0, \omega) \times P_\omega(x - x', z_p)\, P_\omega(y - y', z_p). \tag{7}$$

Here we introduce the partial Kirchhoff propagator for the monochromatic wave,

$$P_\omega(x, z) = (i\lambda z)^{-1/2} \exp\left(i\pi x^2/\lambda z\right), \qquad \lambda = 2\pi c/\omega. \tag{8}$$

The formula (7) is well known in monochromatic theory. In our derivation it was obtained from a property of the Fourier transformation that the product of two functions in k-space corresponds to the convolution of these functions in x-space. The Kirchhoff propagator in k-space has the form

$$P_\omega(k, z) = \exp\left(-i\frac{cz}{2\omega}k^2\right). \tag{9}$$

Thus, we arrive at the conclusion that the propagation of a time-dependent pulse along the optical axis can be successfully calculated in terms of monochromatic waves for which the methods of calculation are well developed. Then the time dependence of the field can be obtained by means of Fourier transformation (6).

2.2. Transmission of an XFEL coherent wave through an object

Let us consider the propagation of the field through an object which is characterized by the complex susceptibility $\chi(\mathbf{r}, t)$ as a space- and time-dependent function. Now we need to consider the next Maxwell equation,

$$\left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) E(\mathbf{r}, t) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} \int dt'\, \chi(\mathbf{r}, t - t')\, E(\mathbf{r}, t'). \tag{10}$$

Here the right-hand side of the equation is proportional to the induced current density which is calculated by a linear approximation over the external field. In our case the angles of scattering are very small; therefore we can neglect the size of scattering centres. This is why the induced current at the point $\mathbf{r}$ is determined by the field at the same point. A detailed analysis of the interaction of X-rays with matter can be found by Afanasev & Kagan (1968). We will find the solution in the form

$$E(\mathbf{r}, t) = \int \frac{d\omega}{2\pi} \exp(-i\omega t + i\omega z/c)\, A(\mathbf{r}, \omega), \tag{11}$$

where $A(\mathbf{r}, \omega)$ is a new function. It is slowly varying in space, and it has a maximum value at very high frequency ω_0. As a rule, the object has a relatively small size L along the optical axis. Taking this into account we neglect second derivatives of $A(\mathbf{r}, \omega)$ over space coordinates because the main change is connected with the first derivative over z. As a result we obtain the approximate equation

$$\frac{\partial}{\partial z} A(\mathbf{r}, \omega) = i(\omega/2c)\, \chi(\mathbf{r}, \omega)\, A(\mathbf{r}, \omega) \tag{12}$$

which has the solution

$$A(x, y, z_1, \omega) = T_O(x, y, \omega)\, A(x, y, z_0, \omega) \tag{13}$$

where $z_1 = z_0 + L$, and

$$T_O(x, y, \omega) = \exp\left[i(\omega/2c) \int_{z_0}^{z_1} dz'\, \chi(x, y, z', \omega)\right]. \tag{14}$$

Finally, we have the next formula for the electric field amplitude,

$$E(x, y, z_1, \omega) = \exp[i(\omega/c)L]\, T_O(x, y, \omega)\, E(x, y, z_0, \omega). \tag{15}$$

The function $T_O(x, y, \omega)$ is called the transmission function. Formula (15) is widely used in monochromatic theory as an approximation for thin optical elements.

In this approximation the longitudinal size L of the object is taken into account only in the phase factor because we neglect the second derivatives over x,y coordinates. However, if we consider a zero object, *i.e.* with $\chi = 0$, then we have to use the formula (7) instead of (15) as it is more accurate. Therefore, in computer simulations we consider the object as having a zero longitudinal size and placed at its middle point. On the other hand, the longitudinal distances in front of and behind the object are increased by $L/2$.

2.3. One-dimensional case

The recurrent formulae (7) and (15) allow one to take into account many various objects located on the optical axis and all free space intervals between them. To simplify the formulae and analysis we shall assume that the objects are homogeneous over the y coordinate. Therefore the transmission function depends only on the x coordinate. In this case the registered intensity has no y-dependence, and we exclude the y coordinate in further derivations. Then the time dependence of XFEL radiation field can be calculated by means of a Fourier integral over a frequency spectrum,

$$E(x, z, t) = \int \frac{d\omega}{2\pi} \exp(-i\omega t)\, E(x, z, \omega), \tag{16}$$

and we have to calculate the propagation of the monochromatic harmonics of the radiation pulse from the source to the detector. Below, to shorten the formulae, we shall omit the index ω.

The transmission function of a double concave parabolic refractive lens can be written in the form

$$T(x, f_c) = \exp\left(-i\pi\frac{x^2}{\lambda f_c}\right), \quad f_c = \frac{f}{1 - i\gamma}, \quad f = \frac{R}{2\delta}, \tag{17}$$

where R is the radius of curvature at the parabola apex (see Fig. 2). The complex susceptibility of the lens material χ is assumed to be homogeneous, and $\chi = -2\delta + 2i\beta$. The parameter $\gamma = \beta/\delta$ is a measure of the focusing. It is modest for X-rays owing to absorption. We note that $\gamma \ll 1$ and sometimes we shall consider a linear over γ approximation.

A real refractive lens has a finite aperture A (see Fig. 2) and equation (17) is valid only for $|x| < A/2$. We consider two cases where the aperture of the lens is not essential. If the aperture is rather large, then the transmission changes the amplitude of

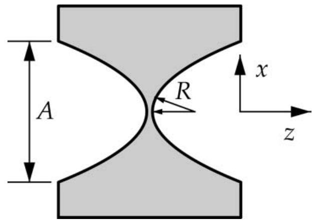

Figure 2
Refractive-lens parameters.

the incident plane wave owing to absorption. In this case the full width at half-maximum (FWHM) of the intensity profile behind the lens is equal to

$$A_\gamma = e_1 \left(\frac{\lambda f}{\gamma}\right)^{1/2}, \qquad e_1 = \left(\frac{2\ln 2}{\pi}\right)^{1/2} = 0.6643. \qquad (18)$$

This value can be considered as an effective aperture of the lens owing to absorption (Snigirev *et al.*, 1996), and the geometrical aperture does not influence the result of the calculation. If this is not the case, and $A_\gamma > A$, then we shall consider the cases where the FWHM of the incoming beam is less than the aperture of the lens. In this case the geometrical aperture does not influence the result, similar to the first case. Below we restrict ourselves by these cases.

We note that in the general case the transmission function (17) is a Gaussian function, *i.e.* it is the exponential of x^2. It is also known that the Gaussian wave propagates in free space without changing its shape. Therefore we can make a general statement that the incoming Gaussian wavefunction of the coherent radiation does not change its shape during propagation through the parabolic lens and propagation in free space over a distance z. Such a process is described by the equation

$$E(x, z_1) = \int \mathrm{d}x' \, P(x - x', z_\mathrm{p}) \, T(x', f_\mathrm{c}) \, E(x', z_0), \qquad (19)$$

which follows from the combined usage of (7) and (15). Here $z_1 = z_0 + z_\mathrm{p}$ and we omit the factor $\exp(i\omega z_\mathrm{p}/c)$ which can be added to the final result.

2.4. Integral over time intensity

It is known that all kinds of X-ray radiation sources create radiation with a pulse structure. The time duration of various coherent pulses can be estimated from the energy spectrum according to the time–energy uncertainty principle $\Delta t \Delta E \simeq h$, where h is Planck's constant and E is the photon energy. A wide spectrum corresponds to a short coherent pulse duration. If the measurement time is longer than the duration of the coherent pulse we can integrate the time-dependent intensity with infinite limits. As a result we have

$$\langle I(x, z) \rangle = \int \mathrm{d}t \left| E(x, z, t) \right|^2 = \int \frac{\mathrm{d}\omega}{2\pi} \left| E(x, z, \omega) \right|^2. \qquad (20)$$

Even in this case, contrary to the monochromatic case, we have to calculate the propagation of all energy harmonics in the registered wavefield. The frequency region of integration is defined mainly by the spectrum of incident radiation from the source, but it can be modified owing to propagation through the system. However, for hard X-rays and the system considered in this work, such a modification cannot be strong. We note that the 0.3 fs duration of a coherent pulse of an XFEL spike is much smaller than the duration of the total pulse, 100 fs. In many experiments with an XFEL it is assumed that a short pulse is of duration 100 fs and consists of many incoherent spikes which propagate simultaneously (EXFEL, 2011). This situation is similar to the case of a synchrotron radiation pulse and an undulator pulse and has only a quantitative, not a qualitative, difference. The coherent pulse of XFEL radiation is longer compared with synchrotron radiation and undulator pulses. Thus, a measurement of the time evolution of the coherent pulse will be impossible in current experiments, although the energy spectrum of XFEL radiation is just determined by the 0.3 fs time duration and the time–energy uncertainty principle.

We note that the same situation takes place in the case of an X-ray tube (Afanasev & Kohn, 1977). The relative energy band $\Delta E/E$ for the characteristic Mo $K\alpha$ radiation is of the order of 3×10^{-4}. Therefore the duration of the coherent pulses of atomic de-excitation is even longer than for XFEL radiation; but the measurement time is much longer.

3. Focusing monochromatic wave: analytical analysis

3.1. Incident wave and general case of *n* lenses

The calculation starts from the wavefunction in front of the first lens. This wavefunction is not known in detail owing to many factors which are difficult to take into account. For example, there may be various optical elements on the initial path of the X-ray beam such as mirrors, monochromators, slits, *etc.* Another reason is the very high speed of the radiating electrons and the subsequent SASE regime. Therefore, instead of taking into account the accurate unknown shape of the wavefunction, we need to use a model approximate shape for obtaining the results of the calculation which describe the experimental results with reasonable accuracy. It is known that the electron radiates a spherical wave in its own coordinate system. At a large distance z_0 each monochromatic component of the wave from the point source, located at x_0, is proportional to $P(x - x_0, z_0)$. As follows from our experience, such a simple model allows the results of many experiments with synchrotron radiation to be described where the spatial width of the beam is not essential. This takes place if the beam is restricted by the slit or pinhole.

In the more general case we need to take into account the spatial structure of the beam. First of all, owing to relativistic effects the spherical wave in its own electron coordinate system is transformed to a wave with finite angular divergence in the laboratory coordinate system. However, it is known that within the beam cone the phase front of the wave remains spherical (parabolic at a large distance). We would like to use the model which was proposed for the first time by Kohn *et al.* (2009). In this model the wavefunction in front of the first lens is described by the same function $P(x - x_0, z_{0\mathrm{c}})$, but with the complex longitudinal coordinate $z_{0c} = z_0 - i\sigma$ under the condition $\sigma \ll z_0$. If α_0 is the angular divergence of the incident-beam intensity (FWHM), then it is easy to show that

$$\sigma = \lambda e_1^2/\alpha_0^2, \tag{21}$$

where e_1 is determined by (18). Substituting the parameters of XFEL, namely λ = 0.1 nm, α_0 = 1 µrad, we obtain σ = 44 m. So the condition $z_0 > \sigma$ can be fulfilled on an XFEL source where z_0 is greater than 500 m. Under the specified condition the angular divergence of the beam is independent of distance, whereas the wavefunction has a form suitable for the calculations (see below). The transverse size of the beam at a distance of 500 m is equal to only 0.5 mm.

Let us consider now an arbitrary lens of our lens system (the first as a particular case) and introduce the most general form for the Gaussian wave as follows (Kohn, 2003),

$$E_0(x, x_0) = T(x, a_0)\, P(x - x_0, b_0)\, T(x_0, c_0), \tag{22}$$

where a_0, b_0, c_0 are the complex parameters, the index 0 means the position on the optical axis (z_0) and

$$\begin{aligned} T(x, a) &= \exp\left(-i\pi\frac{x^2}{\lambda a}\right), \\ P(x, b) &= (i\lambda b)^{-1/2}\exp\left(i\pi\frac{x^2}{\lambda b}\right). \end{aligned} \tag{23}$$

We want to formulate a theorem that the form (22) is conserved on all paths from the first lens to the detector, and only the complex parameters change their values. This change takes the form of relations which can simplify both analytical and numerical calculations of complex optical systems.

Assuming that the wavefunction in front of the lens has the form (22), we substitute (22) into (19) and obtain an integral which looks like a Fourier image of the Gaussian function. A direct calculation can be performed taking into account the well known optical integral

$$\int \frac{\mathrm{d}k}{2\pi}\exp\left(ikx - i\frac{g}{4\pi}k^2\right) = (ig)^{-1/2}\exp\left(i\pi\frac{x^2}{g}\right), \tag{24}$$

which is similar to the Fourier image of the Kirchhoff propagator [see formulae (8) and (9)].

The result of the calculation can be written in the same form,

$$E_1(x, x_0) = T(x, a_1)\, P(x - x_0, b_1)\, T(x_0, c_1), \tag{25}$$

where a_1, b_1, c_1 are the new complex parameters and the index 1 means a position on the optical axis (z_1). The new parameters a_1, b_1, c_1 of the wavefunction at a distance $z_{\rm p}$ behind the lens can be calculated from the initial parameters a_0, b_0, c_0 of the wave (22) by means of the formulae

$$\begin{aligned} &a_1 = d(b_1/b_0), \qquad b_1 = b_0 + z_{\rm p} - (z_{\rm p}b_0/d), \\ &c_1 = c_0/(1 + z_{\rm p}c_0/b_1 d), \qquad d = a_0/(1 + a_0/f_{\rm c}). \end{aligned} \tag{26}$$

The derivation is shown in Appendix *A*. The relations (26) allow one to calculate an optical system consisting of an arbitrary number of refractive parabolic lenses placed with arbitrary distances between them. This is very useful for a fast estimation of the beam parameters transmitted through such a system.

Applying formulae (26) n times for n lenses we obtain a solution at a distance z from the last lens as (25) with the new values of the parameters a, b and c where we have omitted the indices. The intensity is a square modulus of (25). It is useful to consider the relative intensity, *i.e.* divided by the intensity of the incident beam in the case without lenses at the position of the last lens, which is equal to $(\lambda z_{\rm t})^{-1}$ in our case, where $z_{\rm t}$ is the total distance from the source to the last lens. We note that $z_{\rm t}$ does not depend on z. The result can be written as

$$I(x, z, x_0) = \frac{z_{\rm t}}{|b|}\exp\left\{-\frac{[x - x_m(z)]^2}{2\sigma^2(z)}\right\}\exp\left(-\frac{x_0^2}{2\sigma_0^2}\right), \tag{27}$$

where

$$\begin{aligned} &\sigma(z) = \left[\frac{4\pi}{\lambda}(A - B)\right]^{-1/2}, \qquad x_m(z) = -Mx_0, \\ &M = \frac{B}{A - B}, \qquad \sigma_0 = \left[\frac{4\pi}{\lambda}(C - AM)\right]^{-1/2}, \\ &A = -{\rm Im}(a^{-1}), \quad B = -{\rm Im}(b^{-1}), \quad C = -{\rm Im}(c^{-1}). \end{aligned} \tag{28}$$

Equation (27) describes the Gaussian function for all z with FWHM $w(z) = e_2\sigma(z)$ where $e_2 = (8\ln 2)^{1/2} = 2.355$. The position of the beam centre is determined by $x_m(z)$.

Let us consider the general conclusions about the parameters taking into account some evident physical properties of the beam propagation. So, the peak height depends on the z coordinate through $|b|^{-1}$. In addition, it depends exponentially on x_0^2. The latter dependence appears owing to the fact that the ray trajectory from the point source, strongly deviated from the optical axis, cannot pass through the centre of apertures of all lenses. Absorption inside the lens material is a reason for decreasing the intensity maximum. In this way the lens system restricts the effective region of the extended source. It is evident that this property cannot depend on z. We obtain from this conclusion that the quantity $C - AM$ does not depend on z. This property is valid in numerical calculations but it is very difficult to prove analytically.

The intensity integrated over x, $S(x_0) = e_3 w(z) I_m(z, x_0)$, where $I_m(z, x_0) = I(x_m, z, x_0)$ and $e_3 = (4\ln 2/\pi)^{-1/2} = 1.0645$. It is evident from the energy conservation law that it also does not depend on z since we neglect the radiation absorption in air. Considering the source placed on the optical axis we have

$$S(0) = (\lambda/2G)^{1/2}, \qquad G = |b|^2(A - B). \tag{29}$$

Thus, we find that the quantity G does not depend on z. On the other hand, the parameter $M = {\rm Im}(b)/G$ depends linearly on z since b is a linear function of z, as follows from the recurrent formulae (26).

We express $w(z)$ in terms of G as follows,

$$w(z) = e_2(\lambda/4\pi G)^{1/2}|b|. \tag{30}$$

Therefore we see that the z-dependence of the transverse size of the beam is the same as $|b|$, whereas for the peak height it is the same as $|b|^{-1}$. We can write $b = B_0 + zB_1$ where B_0 and B_1

are complex constants which can be determined, for example, just behind the last lens. We call the distance z, where the function $|b|^2$ has the minimum value, the focal distance z_f. It is easy to see that $z_f = -\mathrm{Re}(B_0 B_1^*)/|B_1|^2$.

We note that a compound refractive lens can consist of many elements of various structure. Each element can be considered as a separate lens. Such an approach allows one to perform calculations for a thick lens for which the total lens length is comparable with or even greater than the focal length counted from the last lens.

3.2. Focusing by one lens

Let us consider the simplest case of one thin lens using the recurrent relations described above. A sketch of the geometry is shown in Fig. 3. If the point source is located on the optical axis ($x_0 = 0$) then the coefficient c is out of interest. In front of the lens we have $a = \infty$, $b = z_{0c}$. Just behind the lens we have $a = f_c$, $b = z_{0c}$. Then we obtain in the linear approximation over small parameter γ that $A = \gamma/f$, $B = -\sigma/z_0^2$. The width (FWHM) of the beam is equal to

$$w(0) = \frac{A_\gamma}{(1 - B/A)^{1/2}} = A_\gamma \left(1 + \frac{A_\gamma^2}{A_\alpha^2}\right)^{-1/2}. \qquad (31)$$

Here we have taken into account (18) and (21) and introduce the width (FWHM) of the beam in front of the lens as $A_\alpha = z_0\alpha_0$. If the effective aperture of the lens is less than this width, then the width of the beam will be decreased. In the opposite case it stays the same.

Considering the dependence along the optical axis we obtain

$$B_0 = z_0 - i\sigma, \qquad B_1 = 1 - \frac{z_0}{f} + \frac{i}{f}(\sigma + \gamma z_0). \qquad (32)$$

Neglecting here small imaginary parts we obtain the focus distance as

$$z_f = -\frac{\mathrm{Re}(B_0)}{\mathrm{Re}(B_1)} = \frac{f}{1 - f/z_0}. \qquad (33)$$

The width of the beam at the focus distance

$$w(z_f) = w(0)\left|\frac{b(z_f)}{b(0)}\right| = \frac{w(f)}{|1 - f/z_0|}\left(1 + \frac{A_\gamma^2}{A_\alpha^2}\right)^{1/2}, \qquad (34)$$

where

$$w(f) = \gamma A_\gamma = e_1(\lambda f \gamma)^{1/2} = e_1^2 \lambda f / A_\gamma \qquad (35)$$

is the beam width at the focus in the case of a plane incident wave ($z_0 = \infty$). We note that, for an XFEL, $f \ll z_0$.

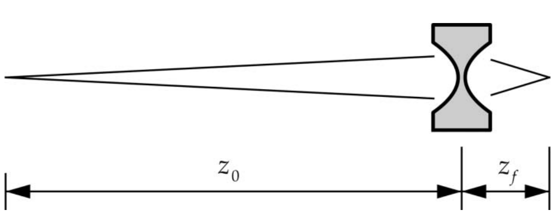

Figure 3
One-lens focusing system.

If the effective aperture of the lens is less than the initial beam size, then the beam size just behind the lens will be decreased by the factor γ which can be considered as a measure of focusing by the refractive lens. In the opposite case the focusing phenomenon is less effective, and for $A_\gamma > A_\alpha \gamma^{-1/2}$ it is absent. The parameter A_γ can be decreased by decreasing the curvature radius R of the lens shape. It may be useful to apply an adiabatic lens (Schroer & Lengeler, 2005) which begins with elements of large effective aperture and continues with elements of decreasing effective aperture together with decreasing the beam size.

3.3. Focusing by two lenses

A system of two lenses is of interest owing to the focusing of a convergent wave by a second lens. To simplify the analysis we assume a plane incident wave for the first lens. In this case the relative wavefunction is described by $(b_0/b)^{-1/2} T(x, a)$ only, but we can use the recurrent relation (26) under the condition $b_0 = \infty$. In addition, we shall assume that two lenses are made from the same material, therefore $\gamma_1 = \gamma_2 = \gamma$. Starting with $a = \infty$ we obtain $a = f_{c1} - z_1$, $b/b_0 = a/f_{c1}$ behind the first lens with complex focal length f_{c1} and just in front of the second lens which is placed at distance z_1 from the first lens (Fig. 4). At a distance z behind the second lens with complex focal length f_{c2} we calculate

$$a = F_c - z\,, \qquad \frac{b}{b_0} = \left(1 - \frac{z}{F_c}\right)\left(1 - \frac{z_1}{f_{c1}}\right), \qquad (36)$$

where

$$F_c = \frac{(f_{c1} - z_1) f_{c2}}{f_{c1} + f_{c2} - z_1}. \qquad (37)$$

Neglecting absorption of X-rays in the lenses, we obtain immediately that the focus distance $z_f = \mathrm{Re}(F_c)$ of the two-lens system, counted from the second lens, satisfies the relation

$$\frac{1}{z_f} = \frac{1}{f_1 - z_1} + \frac{1}{f_2}. \qquad (38)$$

If $z_1 < f_1$ then $z_f < f_2$.

The width of the beam at the focus can be obtained from the imaginary part of F_c calculated in the linear over γ approximation. We can write the FWHM of the beam $w(z_f)$ at the focus in the form

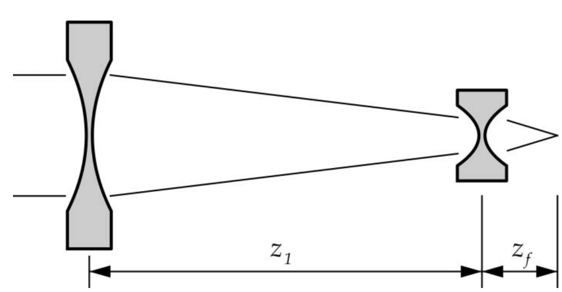

Figure 4
Two-lens focusing system.

$$w(z_{\rm f}) = w_2(f_2)\,\frac{(p+h^2)^{1/2}}{|\,p+h\,|}, \tag{39}$$

where

$$w_2(f_2) = e_1(\lambda f_2\gamma)^{1/2}, \quad p = \frac{f_2}{f_1}, \quad h = 1 - \frac{z_1}{f_1}. \tag{40}$$

Here $w_2(f_2)$ is the beam width at the focus in the case of focusing a plane wave by only the second lens. The calculation is direct and is shown in Appendix *B*.

The peak height of the relative intensity profile $D(z_{\rm f})$ at the focus is equal to (27) with $x = x_0 = 0$, $z_{\rm t} = b_0$ and $z = z_{\rm f}$. We note that $b_0 = \infty$ and $b = \infty$ but their ratio has a sense of the ratio of the focused intensity and plane wave intensity. We obtain

$$D(z_{\rm f}) = \frac{b_0}{|b(z_{\rm f})|} = \frac{|\,p+h|}{\gamma(p+h^2)}. \tag{41}$$

The case of $p \ll 1$ is of interest. Here the first lens has a large aperture, and the second lens gives a small beam size at the focus. For the values of distance z_1 where $h^2 > p$ we find that $z_{\rm f} \simeq f_2$, $w(z_{\rm f}) \simeq w_2(f_2)$, but $D(z_{\rm f}) \simeq 1/(\gamma h)$. Since a normal gain is $1/\gamma$ and $h < 1$ we obtain an increasing gain with decreasing h. In another region, where $h^2 < p$, but $h > p$, the beam size becomes larger by a factor of $p^{1/2}/h$. On the other hand, the gain is equal to $D(z_{\rm f}) \simeq h/(\gamma p)$. Finally, if $h < p$, the beam size and the gain at the focus correspond to the first lens, and the existence of the second lens does not influence the focusing. For negative values of h the picture described above is in the reverse direction. The maximum gain is reached at $h = (p+p^2)^{1/2} - p \simeq p^{1/2}$ for $p \ll 1$. At this distance the beam size in front of the second lens is equal to its effective aperture. The maximum factor of increasing the gain is equal to $1/(2p^{1/2})$, which is two times smaller than the ratio of the effective apertures of the lenses. The main result of our analysis is that the two-lens system cannot make the beam size smaller than the beam size created by the second lens alone, but it can increase the intensity gain. Focusing a convergent beam brings about a larger beam size compared with the parallel-beam case. This analysis is in agreement with computer simulations (Kohn, 2009).

4. Focusing polychromatic beam: computer simulations

The total XFEL pulse of duration 100 fs consists of many short coherent pulses (spikes) of duration 0.3 fs. The width of the energy spectrum of the radiation is determined by the short coherent 0.3 fs pulses, but the measurement time is equal to the full pulse of 100 fs, *i.e.* it is much longer. Under these conditions the results of a theoretical study of the time structure of a coherent pulse of duration 0.3 fs modified by various optics as performed in several works [see Bushuev (2008) and references therein] cannot be measured even with a very fast detector. On the other hand, all conditions of the sample illumination can be described in frequency space for both very fast and very long processes. In the case of focusing optics the main question is what happens with the beam width at the focus in the case of short (non-monochromatic) pulses in the integral over time measurement. It is evident that the best focusing takes place for a monochromated beam. The refractive properties of the lens depend on the frequency. Therefore the focus distance of the lens is different for different frequencies. As a result the beam size at the focus can only be larger for the polychromatic beam compared with the monochromatic beam. In this work we have studied the space properties of the beam modified by the finite energy spectrum of the XFEL radiation.

For the sake of simplicity we will assume that the energy spectrum has a Gaussian shape and is centred at the energy E = 12.4 keV. As for the space part of the incident radiation, it is the same for all energies. We shall consider various relative FWHM $\Delta E/E$. For the European XFEL, $\Delta E/E \simeq 10^{-3}$.

Considering the polychromatic intensity we use the formula (27) for the relative monochromatic intensity with $x_0 = 0$ and multiply it by the incident intensity with a normalized energy dependence of Gaussian shape. As a result we have

$$\langle I(x,z,E)\rangle = \int {\rm d}E_1\,\frac{z_t}{|b(z,E_{\rm c})|}\exp\left[-\frac{x^2}{2\sigma^2(z,E_{\rm c})}\right]G(E_1,\Delta E), \tag{42}$$

where the parameters b, σ and $z_{\rm t}$ are described by (27), (28), $E_{\rm c} = E + E_1 = \hbar\omega$, and

$$G(E_1,\Delta E) = \frac{1}{(2\pi)^{1/2}\sigma_E}\exp\left(-\frac{E_1^2}{2\sigma_E^2}\right), \quad \sigma_E = \Delta E/e_2. \tag{43}$$

We note that $\lambda = hc/E_{\rm c}$ where h is Planck's constant, hc = 1.23984 keV nm.

In the general case it is difficult to calculate the integral (42) analytically because of the complex energy dependence of the parameter γ. Therefore we present the results of a computer simulation for some particular cases in which the parts δ and β of the refractive index are calculated from the table in the `f1f2_Windt.dat` file which is part of the program *XOP-2.0* (XOP, 2011). This table gives the contribution from the photoabsorption process to the atomic scattering factors. In addition, the contribution to β from the inelastic Compton scattering is calculated based on the approximation given in the book by Van Greken & Markowicz (1993). Let us consider the case of one parabolic lens made of Si with radius of curvature R = 1 µm. The other parameters have the following values: z_0 = 500 m, α_0 = 1 µrad, E = 12.4 keV, z = 15.9 cm ($z = f = R/2\delta$ for E = 12.4 keV). We note that the maximum relative intensity just behind the lens is equal to unity whereas at the focus it is approximately equal to $\gamma^{-1} \simeq 100$. Fig. 5 shows the intensity profiles at the focus distance for $\Delta E/E = 0, 10^{-3}$ and 10^{-2}. The first two curves coincide completely and only the third curve has a smaller maximum. Thus, the XFEL pulses will be focused by such a lens as a monochromatic wave. Even for the radiation from an undulator the width of the focused beam will be only slightly wider compared with the monochromatic beam. The FWHM of the focused beam is $w(f)$ = 0.26 µm. The effective aperture is 100 times larger, and it is equal to A_γ = 26 µm. The geometrical aperture must be two times larger than A_γ, *i.e.* A = 52 µm. In this case the total

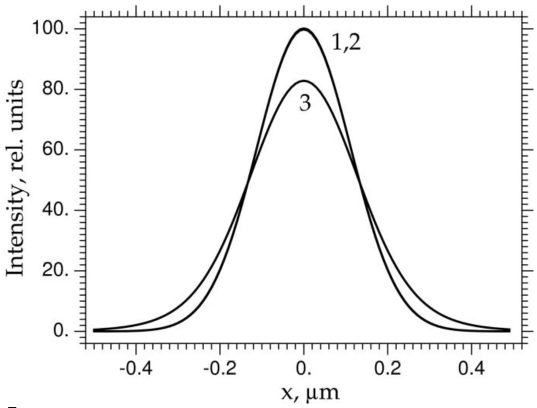

Figure 5
Relative intensity profiles at the focus for a parabolic refractive lens made from Si, with the curvature radius R = 1 μm, for E = 12.4 keV, and $\Delta E/E$ = 0 (curve 1), 10^{-3} (curve 2) and 10^{-2} (curve 3). Curves 1 and 2 completely coincide with each other and have a maximum of 100. See text for more details.

length of the lens $L = A^2/4R = 0.68$ mm. It is much smaller than the focal distance.

Let us consider a nanofocusing lens with $L \simeq f/2$ and $A \simeq 2A_\gamma$. Such a lens must have a radius of curvature of R = 0.01 μm, then f = 1.59 mm, A_γ = 2.6 μm, $w(f)$ = 26 nm. We note that for decreasing the focus width by ten times it is necessary to decrease the curvature radius and the focus distance by 100 times. The calculation shows the same intensity profiles as shown in Fig. 5 but with the scale of the x axis ten times smaller; therefore the FWHM is 26 nm instead of 0.26 μm, but the height of the maximum is the same. This fact can be explained as follows. We variate the energy inside the interval with small relative energy values. Such values correspond to small relative values of the parameters b and σ in (42). Therefore the parameters which influence the shape of the curves can be used in the linear approximation in the expansion over $\Delta E/E$. As a result, their absolute change is proportional to the values for the middle energy. For example, ΔE brings about Δf, but $\Delta f/f$ is proportional to $\Delta E/E$. So decreasing f leads to a decreasing Δf and the same for the focus width. It is clear that under such conditions the shape of the curves at the focus is invariant in the proper scale of the x axis.

5. Conclusion

The coherent pulse duration of the European XFEL (0.3 fs) is much smaller than the measuring time which is larger than the full pulse duration (100 fs). Therefore we need to calculate the integral of the coherent pulse intensity over time. This intensity can be alternatively calculated as the integral over the spectrum intensity for the monochromatic wave. We show that for a parabolic lens system a semi-analytical method of calculation can be useful, in which the Gaussian shape of the wavefield is conserved and only three parameters are needed for the calculation. Our calculations show that an energy spectrum with relative width $\Delta E/E = 10^{-3}$ does not influence the monochromatic focus property. Finally we can conclude that the refractive optics can focus XFEL pulses completely, *i.e.* as for a monochromatic wave. An additional monochromator is not necessary. This is different from the conclusion made in TDR (2007).

APPENDIX *A*
Derivation of formula (26)

We substitute (22) into (19), replace x' by k, and obtain the integral as follows,

$$E_1(x, z_1) = \frac{2\pi \exp(i\alpha)}{i\lambda(z_{\rm p} b_0)^{1/2}} \int \frac{{\rm d}k}{2\pi} \exp\left(iks - i\frac{g}{4\pi}k^2\right), \qquad (44)$$

where

$$\alpha = \frac{\pi}{\lambda}\left[\frac{x^2}{z_{\rm p}} + x_0^2\left(\frac{1}{b_0} - \frac{1}{c_0}\right)\right],$$
$$s = -\frac{2\pi}{\lambda}\left(\frac{x}{z_{\rm p}} + \frac{x_0}{b_0}\right), \qquad g = -\frac{4\pi^2}{\lambda}\frac{b_1}{z_{\rm p} b_0}. \qquad (45)$$

Here b_1 is determined by (26). Then we apply formula (24) for the integral and replace the integral by the right-hand side of (24). We obtain the result as a product of pre-exponential and exponential factors. In calculating the first term we choose the root $(-1)^{-1/2} = i$ for convenience. We note that the constant phase factor in the wavefield amplitude does not influence the intensity. Then it is easy to calculate the pre-exponential factor as $(i\lambda b_1)^{-1/2}$.

The exponential factor

$$\exp\left(i\alpha + i\pi\frac{s^2}{g}\right) = \exp\left\{i\pi\left[\frac{(x - x_0)^2}{\lambda b_1} - \frac{x^2}{\lambda a_1} - \frac{x_0^2}{\lambda c_1}\right]\right\}, \qquad (46)$$

where a_1 and c_1 are determined by (26). The latter formula can be verified by direct calculation.

APPENDIX *B*
Derivation of formula (39)

We note that in our case $w(z_{\rm f}) = e_2\sigma(z_{\rm f}) = e_1[\lambda\,{\rm Im}(F_{\rm c})]^{1/2}$. It follows from (28) because $e_1 = e_2(4\pi)^{-1/2}$, $B = 0$ when $b = \infty$, $A = [{\rm Im}(F_{\rm c})]^{-1}$ because ${\rm Re}(F_{\rm c} - z_{\rm f}) = 0$. We need to calculate ${\rm Im}(F_{\rm c})$ from (37) in the linear over γ approximation. Applying notation (40) we have

$$F_{\rm c} = f_2\frac{(h + i\gamma)(1 + i\gamma)}{(h + p + i\gamma(1 + p))}. \qquad (47)$$

In the linear over γ approximation we find finally

$${\rm Im}(F_{\rm c}) = f_2\gamma\frac{p + h^2}{(p + h)^2}. \qquad (48)$$

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