Specific properties of X-ray compound refractive lens. Theoretical analysis

V. Kohn, I. Snigireva¹ and A. Snigirev¹

Russian Research Centre "Kurchatov Institute", 123182 Moscow, Russia ¹ European Synchrotron Radiation Facility, BP 220, 38043 Grenoble cedex, France

Abstract. We present the diffraction theory for the x-ray compound refractive lens (XCRL) operation as an imaging device in the paraxial approximation. We obtain the analytical expression for the image propagator in the case of parabolic XCRL that allows us to explain the peculiarities of imaging and focusing with the XCRL observed previously in the experiments. We propose the enhanced thin lens formula for the relatively long XCRL with the longitudinal size *L* taking into account the linear corrections in L/F where *F* is the focal length in the thin lens approximation. A relatively small aperture of XCRL due to absorption of x rays limits the resolution and, in addition, leads to phase effects visualizing the local phase gradient of the radiation wave field produced by transparent objects. This opens novel technique of imaging for purely phase objects, which is different from the in-line phase contrast imaging techniques.

1. INTRODUCTION

Since the first demonstration [1] of the x-ray compound refractive lens (XCRL) for focusing a synchrotron radiation beam, the x-ray refractive optics is under extensive development. There are successful attempts to develop the refractive optics by means of various approaches. The XCRL with a parabolic profile of surfaces is more promising [2-5]. Unlike visible optics, collecting XCRL has a concave shape and the material of the lens is always absorbing. The latter leads to a significant limitation of the effective aperture a_{γ} which is smaller than the physical transverse size a of the XCRL. This property influences the XCRL operation as an imaging device. The XCRL has a rather large longitudinal size L, therefore the thin lens approximation must be verified. In most practical cases XCRL satisfies the condition L/F << 1, where F is the focal length in the thin lens approximation, so that the linear corrections in L/F are sufficient.

In this work we present the diffraction theory for the parabolic planar (1D) XCRL in paraxial approximation. We solve the parabolic wave equation in terms of propagators. We calculate analytically the intermediate convolutions and obtain the image propagator which connects straightforwardly the wave field $A_o(x)$ at the plane just after the object and the wave field $A_i(x)$ at the image (detector) plane . Due to a relatively small effective aperture of the XCRL the image propagator stays the gauss function of finite width instead of the delta-function. This leads to developing phase or edge enhanced imaging effects, which make visible transparent objects at the image plane. We found out that these edge-enhanced images are associated with the local phase gradient of the wave field $A_o(x)$. Moreover, these images are sensitive to the sign of the phase gradient. This opens quite a new technique of microimaging for purely phase objects, which is different from the traditional phase contrast microimaging techniques.

2. DERIVATION OF THE IMAGE PROPAGATOR

We consider the in-line experimental setup. A fragment of the setup is shown schematically in the Fig. 1(*a*). For the sake of simplicity we restrict ourselves to the case of planar XCRL as an array of chips with a parabolic profile of surface along the *x*-axis and consider two-dimensional space (*x*, *z*). Substituting the wave field strength as $E(x,z) = \exp(ikz) A(x,z)$ into the Maxwell's wave equation, where $k = 2\pi/\lambda$ is a wave

JOURNAL DE PHYSIQUE IV

number, λ is a wave length and applying the paraxial approximation, we arrive to the parabolic equation for A(x,z) inside the XCRL as

$$\frac{dA(x,z)}{dz} = -ik\eta(x)A(x,z) + \frac{i}{2k}\frac{d^2A(x,z)}{dx^2}, \quad \eta(x) = 1 - n(x) = \frac{c}{L}\left\lfloor\frac{x^2}{2F} + \delta dN\right\rfloor, \quad c = 1 - i\gamma, \quad \gamma = \frac{\beta}{\delta}$$
(1)

where we took into account that the length of the individual chip $p = L/N = a^2/4R + d$ is very short compared to the interaction length $L_{int} = 1/k\delta$ and made an averaging of the equation within the distance p, so that the z-dependence of the complex refractive index n(x,z) vanishes. Here δ is a decrement of refractive index, β is an index of absorption of the XCRL material, N is a number of the chips in XCRL, $F = R/2N\delta$ is the focal length of XCRL in the thin lens approximation. The parameters L, R, a and d are shown in the Fig. 1.



Figure 1. Geometrical parameters of the experimental setup (a) and of individual refractive lens chip (b).

Outside the XCRL, i. e. in the free space on the distances r_0 (between the object plane and XCRL) and r_i (between the XCRL and the image plane) we have the same equation where $\delta = \beta = 0$. A general solution of such equation $A(x,z) = P(x - x_0, z) * A_0(x_0)$ can be written as a convolution of the boundary wave field $A_0(x)$ and the propagator $P(x,z) = (i\lambda z)^{-1/2} \exp(i\pi x^2/\lambda z)$ where z is counted from the boundary plane. Inside the XCRL in the zero approximation in L/F we can neglect the second term in the right-hand side of eq.(1). Then we obtain the XCRL propagator as $P_1(x - x_0, z) = \exp[-ik\eta(x)z]\delta(x - x_0)$ where δx is the Dirac delta-function. Such expression is completely equivalent to the thin lens approximation. To simplify the problem let us consider first this case.

The propagators allows one to obtain immediately the solution of the problem, namely, a connection between the image wave field $A_i(x_i)$ and the object wave field $A_o(x_o)$ via the image propagator

$$A_{i}(x_{i}) = G(x_{i}, x_{o}) * A_{o}(x_{o}), \quad G(x_{i}, x_{o}) = P(x_{i} - x_{b}, r_{i}) * P_{i}(x_{b} - x_{f}, L) * P(x_{f} - x_{o}, r_{o})$$
(2)

Here and above the (*) sign means the convolution, namely, the integration over the doubly repeated arguments. In our case all integrals can be calculated analytically because the arguments of exponentials contain x only up to second degree. As a result, we obtain the expression for the image propagator as

$$G(x_i, x_o) = \frac{C_0}{(i\lambda r_g)^{1/2}} \exp\left(i\frac{\pi}{\lambda r_g} \left[g_i x_i^2 - 2x_i x_o + g_o x_o^2\right]\right), \ r_g = r_i + r_o - c\frac{r_i r_o}{F}, \ g_i = 1 - c\frac{r_o}{F}, \ g_o = 1 - c\frac{r_i}{F}$$
(3)

Here the factor $C_0 = \exp(-ik \delta c dN)$ takes into account the phase shift and absorption on the thin part of the chips. We note that the XCRL length L is neglected in this approximation compared to the long distances r_o and r_i .

To obtain the corrections linear in L/F for the XCRL propagator one needs to solve eq.(1) taking into account the second term in the right-hand side. This may be done iteratively. Namely, the solution must be searched in the exponential form. Then on the first iteration one may use in the second term of the equation for the complex phase the solution obtained on the zero iteration and so on. Such approach was

considered for the first time in [6]. The detailed analysis will be published elsewhere [7]. The result can be formulated as follows. The expression (3) for the image propagator remains in the approximation linear in L/F. However, the factor C_0 is multiplied by $\exp(cL/4F)$ due to convergence of rays inside the XCRL. The distances $r_{o,i}$ must be replaced by $r_{o,i} + L/2$. This means that the long XCRL can be treated as the thin lens placed at the middle of the real lens. In addition to this evident correction, the focal length F of such lens must be replaced by F + L/6. Such a correction may be important for the imaging of small oblect, for example, for the imaging of synchrotron radiation source. Below we remain the old notation but keep in mind the corrections pointed above.

3. THE DIFFRACTION THEORY OF THE FOCUSED IMAGE

As is known in the visible optics the focused image occurs when the lens formula $1/r_o + 1/r_i = 1/F$ takes place. Applying this relation to the expression (3) we obtain

$$G(x_{i}, x_{o}) = \frac{C_{0}}{i} \left(\frac{r_{o}}{r_{i}}\right)^{1/2} \exp\left(i\frac{\pi}{\lambda} \left[\frac{x_{i}^{2}}{r_{i}} + \frac{x_{o}^{2}}{r_{o}}\right]\right) \delta_{\sigma}(x_{o} - x_{oi}), \quad \delta_{\sigma}(x) = \frac{\exp(-x^{2}/2\sigma^{2})}{\sigma(2\pi)^{1/2}}, \quad \sigma = \frac{\lambda r_{0}}{a_{\gamma}(2\pi)^{1/2}}$$
(4)

where $a_{\gamma} = (\lambda F/\gamma)^{1/2}$ is the effective aperture of the XCRL, $x_{oi} = -x_i(r_o/r_i)$ is the object point corresponding to the image point. We note that $\delta_{\sigma}(x)$ is the normalized gauss function which becomes the Dirac delta-function $\delta(x)$ in the limit $\sigma \to 0$. Of course, σ decreases when the aperture a_{γ} increases. However, for XCRL the aperture is limited due to absorption and it can not be large even if the geometrical aperture of the XCRL will be large. The aperture decrease occurs simultaneously with the focal distance decrease.

To illustrate how the finite aperture of the XCRL influences the images, let us consider the transparent object illuminated by plane wave when the object function $A_o(x_o) = \exp[i\psi(x_o)]$. Let the phase profile $\psi(x_o)$ have the finite derivatives $\xi_n(x_o) = d^n \psi/dx_o^n$. Since the effective region of integration in (2) has a size σ near the point x_{oi} for the given image coordinate x_i , we can expand the phase in Taylor's series at the point x_{oi} and restrict ourselves only by first three terms, namely, $\psi(x_o) \approx \psi(x_{oi}) + \xi_1(x_{oi})(x_o - x_{oi}) + (1/2) \xi_2(x_{oi})(x_o - x_{oi})^2$. In this case the image function is expressed analytically as

$$A_{i}(x_{i}) \approx \frac{C_{0}}{i} \left(\frac{r_{o}}{r_{i} p_{o}(x_{oi})} \right)^{1/2} \exp \left(i\pi \frac{x_{i}^{2}}{\lambda F} \frac{r_{o}}{r_{i}} - \pi \frac{[x_{oi} + X(x_{oi})]^{2}}{a_{\gamma}^{2} p_{o}(x_{oi})} \right), \quad X(x) = \frac{\lambda r_{o}}{2\pi} \xi_{1}(x)$$
(5)

where $p_o(x) = 1 - i\gamma r_o / F - i\xi_2(x)\sigma^2$.

First of all, this expression shows that if even the object function is constant, i. e. $\xi_1 = \xi_2 = 0$, the image function is not constant. In the typical case when $\gamma r_o \ll F$ the intensity at the image plane is distributed according to the gauss function with the FWHM = 0.66 $a_\gamma(r_i/r_o)$. This means that the XCRL with a finite aperture can not image a large object of size $s > a_\gamma$ in a whole but shows only a fragment of such object with the size of order a_γ . A similar effect exists in the visual optics. It can be explained in the frame of geometrical optics. Indeed, the point of image is the intersection point of many rays. One of them goes from the point of object through the lens center and does not depend on the aperture. There is another ray which is parallel to the optical axis before the lens. The latter ray must go through the aperture as well to obtain the focused image.

We note that within the effective image region both the second and the first derivatives of the object phase profile influence the image intensity profile. However, the role of the second derivative is modest, if $|\xi_2(x_{oi})\sigma^2| \ll 1$. On the contrary, the role of the first derivative in the formation of the object image is significant. When $[x_{oi} + X(x_{oi})]^2 > x_{oi}^2$, the image intensity decreases compared to the background (dark image). The bright image can be observed in some places where the opposite condition is fulfilled. Of course, when $[x_{oi} + X(x_{oi})]^2 = x_{oi}^2$, the image is determined by the second derivative alone. In the latter case the intensity differs slightly from the background value.

This result demonstrates that the XCRL is an excellent device for imaging of transparent objects. However, it shows the image, which is qualitatively different from the image obtained with the in-line setup under the near field condition [8]. The latter technique corresponds formally to eqs.(2),(3) with $C_0 = 1$, $r_o = 0$, $F = \infty$. In this case the propagator is near to $\delta(x_i - x_o)$ for $r_i \rightarrow 0$.

To illustrate the analytical result, we performed the computer simulation for the silicon grid with the period 20 µm, bar height h = 10 µm, bar width 10 µm. We choose the x-ray energy E = 20 keV, the distance $r_s = 50000 \text{ m}$ between the point source and the object, the aluminium XCRL, F = 1 m, $r_o = r_i = 2 \text{ m}$. The very long distance r_s is selected to eliminate some small extra oscillations due to divergence of the beam. However, the divergence does not influence the result which remains practically the same for $r_s = 50 \text{ m}$. The refractive index parameters are: $\delta = 1.352 \times 10^{-6}$, $\beta = 4.21 \times 10^{-9}$, $\gamma = 3.12 \times 10^{-3}$ for Al and $\delta = 1.21 \times 10^{-6}$, $\beta = 4.72 \times 10^{-9}$ for Si. Under these conditions $\sigma = 0.35 \text{ µm}$. The grid can be rotated around the y-axis by the angle θ . The rotation replaces the rectangular phase profile by the trapezoidal phase profile with the width of transition layer $h\sin\theta$. The phase shift on the bar is equal to $|\psi| = 1.22$.



Figure 2. The images of the silicon grid for the rotation angle $\theta = 0$ (*a*) and 10° (*b*), see text for details.

The results of calculation are shown in Fig. 2. The top figures show the near field phase contrast images on the distance 5 cm from the object. The bottom figures show the XCRL images. One can see that the computer simulation confirms the features of the XCRL imaging discussed above analytically. Note that the XCRL image shows always the region of the phase gradient in the contrary to the near field phase contrast image. In addition, the XCRL image is sensitive to the sign of the phase gradient. As for the abrupt phase shift, it can be seen as distinct image with the XCRL resolution. These properties mean more single-valued and direct solution of the phase retrieval problem.

References

- [1] Snigirev A., Kohn V., Snigireva I. and Lengeler B., Nature 384 (1996) 49-51
- [2] Lengeler B., Schroer C.G., Richwin M. and Tummler J., Appl. Phys. Lett. 74 (1999) 3924-3926
- [3] Lengeler B., Schroer C., Tummler J., et al. J. Synchr. Rad. 6 (1999) 1153-1167
- [4] Aristov V., Grigoriev M., Kuznetsov S., et al. Appl. Phys. Lett. 77 (2000) 4058-4060
- [5] Aristov V.V., Grigoriev M.V., Kuznetsov S.M., et al. Opt. Commun. 177 (2000) 33-38
- [6] Snigirev A., Kohn V., Snigireva I, Souvorov A. and Lengeler B., Appl. Opt. 37 (1998) 653-662
- [7] Kohn V., Snigireva I. and Snigirev A., Opt. Commun. (2002) accepted.
- [8] Snigirev A., Snigireva I., Kohn V., Kuznetsov S., Schelokov I., Rev. Sci. Instr. 66 (1995) 5486-5492