Application of the probability theory in predicting 3D focusing behaviors of compound X-ray refractive lenses

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A theoretical m ethod based on the diffractive theory is used for predicting three-dimensional (3D) focusing performances of the compound X-rays refractive lenses (CRLs). However, the derivation of the 3D intensity distribution near focus for the X-ray refractive lenses is quite complicated. In this paper, we introduce a simple theoretical method that is based on the first and second moments in the theory of probability. As an example, the 3D focusing performance of a CRL with Si material is predicted. Moreover, the results are compared with those obtained by the diffractive theory. It is shown that the method introduced in this paper is accurate enough.

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X-rays promise a high resolving power due to the very short wavelength. Therefore, people have been trying to develop X-ray optical devices for focusing X-ray beam to a small spot to perform X-ray analysis techniques. In 1996, Snigirev *et al.*[1] proposed and demonstrated that X-ray refractive focusing could be accomplished with a compound X-ray refractive lens (CRL). And then many publications on the further researches appeared[2−8]. The theoretical results on the focusing performances in the focal plane and the transmission efficiency of CRLs have been presented[2−5]. However there has been little written concerning the three-dimensional (3D) focusing behavior of such a device. In order to obtain a fuller knowledge of the focusing performances of CRLs, the X-ray distribution not only in the focal plane but also in the neighborhood of this plane must be studied. A theoretical method based on the diffractive theory for 3D focusing behaviors of CRLs has been reported[9], however the derivation of the 3D X-ray intensity distribution near focus is quite complicated. It is also not easy to clear up the dependence of the intensity distribution near focus on the structural parameters of CRLs. In the present paper, the authors introduce a simple theoretical method that is based on the first and second moments in the theory of probability for evaluating the 3D focusing behaviors of the device. As a special application, the 3D X-ray intensity distribution near the focus is derived for the CRLs with plano-concave elementary lenses. The relationship between the transverse and axial focusing behaviors is considered and a simple calculation that predicts the transverse and axial focusing behaviors of the device is also presented. The theoretical method introduced in this paper can be easily generalized to other lenses with different structures such as the lenses with double-concave elementary lenses. Moreover, the computer codes based on our theoretical method are developed, and the 3D focusing performance of a Si CRL is predicted and compared with the results by diffractive theory.

Suppose the elementary lenses of a CRL have plano-concave shape (see Fig. 1), where R stands for the radius of the concave surface, d and t are the center thickness and the edge thickness of the elementary lens respectively. When the incident plane monochromatic wave propagates through the elementary lens at an arbitrary point within its aperture, the thickness function[10] $D(r)$ is defined as

$$D(r) = d + R - \sqrt{R^2 - r^2} = d + r^2/2R + O(r) \approx d + r^2/2R, \quad (1)$$

where $O(r)$ stands for the term omitted from the binomial expansion of the square root. Here we should note that Eq. (1) amounts to the approximation of the spherical surfaces of the lens by parabolic surfaces. For the usual paraxial approximation, our theoretical method can be accurate enough.

Now considering a CRL composed of a group of N elementary lenses positioned in line with axial symmetry, the diffractive screen function of the device can be defined as[3]

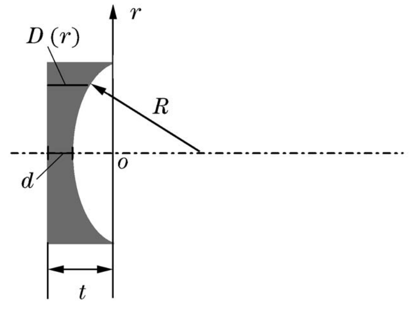

Fig. 1. Scheme of an elementary lens of the compound X-ray refractive lenses.

$$\left\{\begin{array}{l} H_N(r) = C_1 \exp\left[-\frac{2\pi\beta N r^2}{\lambda R}\right] \exp\left[-i\frac{\pi\delta N r^2}{\lambda R}\right] \\ C_1 = \exp\left[-\frac{4\pi\beta dN}{\lambda}\right] \exp\left[i\frac{2\pi}{\lambda}(t-\delta d)N\right] \end{array}\right., \quad (2)$$

where λ stands for the wavelength of incident X-ray radiation, β and δ are related to absorption and refraction respectively in the expression ($\tilde{n} = 1 - \delta - i\beta$) of the optical constant in X-ray region.

According to Kirchhoff integral within the Fresnel approximation[11] and using the diffraction screen function we defined, the complex amplitude of the point (ρ, z) in the image region can be expressed as

$$U(\rho, z) = C_1 C_2 \int_0^\infty \exp\left(-\frac{2\pi\beta N r^2}{\lambda R}\right) \times \exp\left[i\frac{\pi r^2}{\lambda}\left(\frac{1}{z} - \frac{\delta N}{R}\right)\right] J_0\left(\frac{2\pi}{\lambda z} r\rho\right) r\mathrm{d}r, \quad (3)$$

where z is the coordinate along the optical axis, r and ρ stand for the points at the object plane and receiving plane in the image region, respectively. In addition, C_2 in Eq. (3) stands for a constant in Kirchhoff integral equation and J_0 is used to express the first kind Bessel function of order zero. It is obvious therefore from Eq. (3) that the axial and transverse behaviors are not independent. By means of some complicated mathematical derivations[9], the normalized 3D X-ray intensity distribution near focus is

$$\frac{I(\rho, \Delta z)}{I(0,0)} = \frac{64\pi^4\beta^4 N^4 + 16\pi^2\beta^2 N^2 \lambda^2 R^2 \nu^2}{\left[8\pi^2\beta^2 N^2 + 2\lambda^2 R^2 \nu^2\right]^2} \times \exp\left[-\frac{\pi\beta\lambda N R \alpha^2}{4\pi^2\beta^2 N^2 + \lambda^2 R^2 \nu^2}\right], \quad (4)$$

where $\alpha = \frac{2\pi\rho}{\lambda f} = \frac{2\pi N\delta}{\lambda R}\sqrt{x^2+y^2}$, $\nu = \frac{\pi(\Delta z)}{\lambda f^2} = \frac{\pi N^2\delta^2}{\lambda R^2}(\Delta z)$, and $\Delta z = f - z$.

From Eq. (4), some general information on the intensity distribution near focus and the focusing behavior of the CRL can be seen. However, the mathematical derivation is quite complicated, in addition it is not easy to clear up the dependence of the intensity distribution near focus on the parameters of the lenses. Therefore, a simple theory based on the probability theory is worked out for predicting the focal behavior of the CRLs.

For small distances from the focus, we can calculate the focal-plane and the axial X-ray intensity distributions separately[11,12]. So far as the focal-plane X-ray intensity distribution is concerned, we have $\Delta z = z - f = 0$, therefore Eq. (3) can be predigested as

$$U(\rho, 0) = C_1 C_2 \int_0^\infty \exp\left[-\frac{2\pi\beta N r^2}{\lambda R}\right] J_0\left(\frac{2\pi\rho}{\lambda f} r\right) r\mathrm{d}r. \quad (5)$$

For expanding Eq. (5) as a power series by using the definition of Bessel function, we get

$$U(\rho, 0) = \frac{C_1 C_2}{2}\int_0^\infty P(t)\left\{1 - \frac{\alpha^2 t}{4} + \frac{\alpha^4 t^2}{2^4\cdot 2^2}\cdots\right\}\mathrm{d}t \approx \frac{C_1 C_2}{2}\left(M_0 - \frac{\alpha^2}{4}M_1 + \frac{\alpha^4}{64}M_2\right), \quad (6)$$

where α has the same expression with Eq. (4), $P(t) = \exp\left[-2\pi\beta N t/\lambda R\right]$ and $M_n = \int_0^\infty P(t) t^n \mathrm{d}t$, in which $P(t)$ is related to the diffractive screen function, M_n stands for the nth moments of the diffractive screen function. Therefore the normalized X-ray intensity distribution in the focal plane can be expressed approximately as

$$I_N(\rho, 0) = 1 - \frac{\alpha^2}{2}\left(\frac{M_1}{M_0}\right). \quad (7)$$

Using the same reasoning, as far as the axial X-ray intensity distribution is concerned, we have

$$U(0, \Delta z) = C_1 C_2 \int_0^\infty \exp\left[-\frac{2\pi\beta N r^2}{\lambda R}\right] \exp\left[i\frac{\pi r^2}{\lambda f^2}\Delta z\right] r\mathrm{d}r. \quad (8)$$

For expanding Eq. (8) as a power series by means of $\exp(x) = \sum_{n=0}^{\infty}\frac{x^n}{n!}$, the normalized axial X-ray intensity distribution can finally be expressed as

$$I_N(0, \Delta z) = 1 - \nu^2\left[\frac{M_2}{M_0} - \left(\frac{M_1}{M_0}\right)^2\right], \quad (9)$$

where ν has the same expression with that in Eq. (4). Considering of the CRL described in this paper, the zeroth, first, and second moments of $P(t)$ are calculated as

$$M_0 = \frac{\lambda R}{2\pi\beta N}, \quad M_1 = \left(\frac{\lambda R}{2\pi\beta N}\right)^2, \quad M_2 = 2\left(\frac{\lambda R}{2\pi\beta N}\right)^3. \quad (10)$$

Substituting Eq. (10) to Eqs. (7) and (9), we finally get the expressions of the normalized transverse and axial X-ray intensity distributions

$$\left\{\begin{array}{l} I_N(\rho, 0) = 1 - \frac{\pi\delta^2 N}{\lambda R\beta}\rho^2 + \cdots \\ I_N(0, \Delta z) = 1 - \frac{\delta^4 N^2}{4R^2\beta^2}(\Delta z)^2 + \cdots \end{array}\right.. \quad (11)$$

From Eq. (11), we can see that both the transverse and the axial focusing performances of the CRL are relative to the parameters of the lens including its working wavelength (λ), lens material (β and δ), and the structural parameters of the lens such as the number of elementary lenses (N) and the radius of concave surface (R).

Because the low-Z materials are considered to be more suitable for the CRLs with high-energy X-rays (> 5 keV), and Si compound refractive lens is easy to fabricate by standard micro-fabrication techniques, here we choose Si as an example material for predicting 3D focusing performances of CRL theoretically. In order to compare the results with those obtained by the diffractive theory[9], we predict the performances of the same Si CRL. Its parameters are working wavelength of 0.04 nm (the X-ray

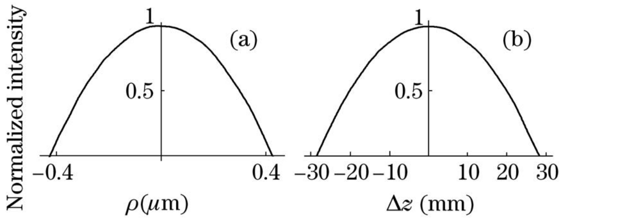

Fig. 2. The normalized transverse and the axial intensity distribution for Si compound X-ray refractive lens. Normalized transverse (a) and axial intensity distributions (b) for Si CRL with $\lambda = 0.04$ nm, $R = 500$ μm, $N = 100$.

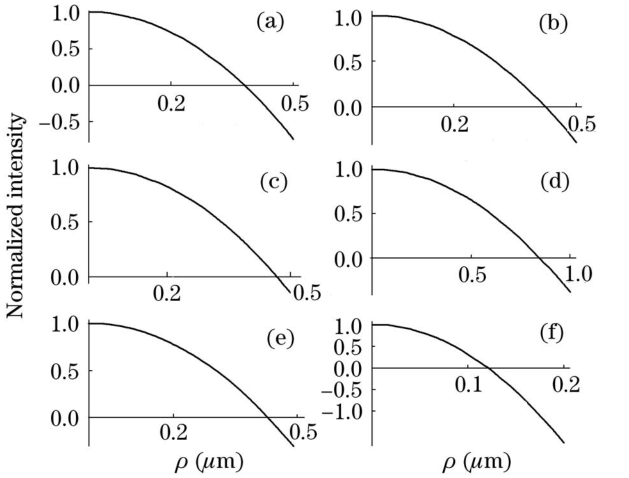

Fig. 3. Normalized transverse X-ray intensity distribution varies with the structure parameters R (in (a), (b), (c), $N = 100$), and N (in (d), (e), (f), $R = 500$ μm). (a) $R = 400$ μm; (b) $R = 500$ μm; (c) $R = 600$ μm; (d) $N = 50$; (e) $N = 100$; (f) $N = 350$. $\lambda = 0.04$ nm.

energy of 29.78 keV), geometrical aperture of 1 mm, the length of the compound lens of around 50 mm, and the focal length of the lens of 9.9 m. According to the theoretical method introduced in this paper, the normalized transverse and axial intensity distributions are calculated and shown in Figs. 2(a) and (b), respectively. From Fig. 2(a), we can see that the full-width at half-maximum (FWHM) of the normalized transverse intensity distribution is around 0.6 μm. A close result (around 0.67 μm) was obtained by the method based on the diffractive theory[9]. In addition, FWHM of the normalized axial intensity distribution is around 44 mm, which is also close with the result (about 50 mm) obtained by the diffractive theoretical method.

In order to clear up the dependence of the intensity distribution near focus on the structural parameters of the CRLs, the normalized transverse intensity distributions are calculated for variable structural parameters R and N. The results calculated for the Si CRL with the X-ray wavelength of 0.04 nm are shown in Fig. 3. It can be seen that the focusing performance is improved as the number of the elementary lenses becomes larger and the parameter R becomes smaller. Moreover, the focusing performances for different X-ray wavelength of 0.15, 0.08, and 0.04 nm are predicted (see Fig. 4). We can see from Fig. 4 that the focal spot becomes smaller when the X-ray wavelength is getting smaller. That means the transverse focusing performance is better when the radiation energy is getting larger.

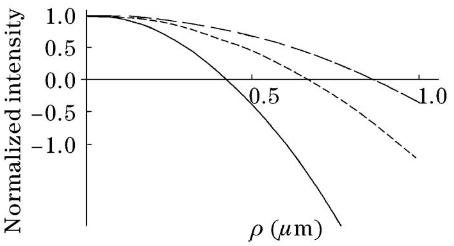

Fig. 4. Normalized transverse intensity distribution for X-ray wavelengths of 0.04 (solid line), 0.08 (dense dashed), and 0.15 nm (sparse dashed), Si compound lens, $R = 500$ μm, $N = 100$.

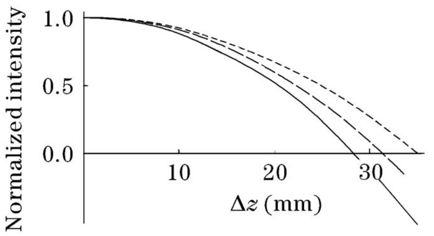

Fig. 5. Normalized axial intensity distribution for X-ray wavelengths of 0.04 (solid line), 0.08 (dense dashed), and 0.15 nm (sparse dashed), Si compound lens, $R = 500$ μm, $N = 100$.

As far as the tolerance in the setting of the receiving plane in an X-ray image-forming system is concerned, the normalized axial X-ray intensity distributions are calculated for the X-ray wavelength of 0.15, 0.08, and 0.04 nm, respectively (see Fig. 5). The result shows that the tolerance in the setting of the receiving plane varies slowly when the X-ray radiation energy changes.

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