Simulation of x-ray transmission through an ellipsoidal capillary

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This paper develops a simulation program for x-ray transmission in an ellipsoidal capillary based on a ray-tracing method. The influence of the parameters of ellipsoidal capillary and x-ray energy on transmission efficiency, full width at half maximum and power density gain of x-ray beams through an ellipsoidal capillary was analysed by this program. It shows that the particular rules of the ellipsoidal capillary x-ray lens are different from the polycapillary lens. Furthermore, this analysis method can be applied to the optimized design of ellipsoidal capillary.

Keywords: ellipsoidal capillary, transmission efficiency, power density gain, simulation

PACC: 0290, 0785

1. Introduction

Hollow glass mono-capillary used to focus synchrotron radiation can be divided into two major categories: multi-bounce capillaries and single-bounce capillaries. As multi-bounce capillaries, tapered capillaries can focus x-rays into the minimum beam size. Tapered mono-capillary optic is a very simple device that has been used in synchrotron radiation for several years.[1−3] However, in order to get smaller beam sizes, the distance between the end of the capillary and the sample is very short; in other words, the tapered capillary has a short working distance. Ellipsoidal capillary, a single-bounce capillary, can focus x-rays with a larger working distance and has a greater transmission efficiency. Until now, ellipsoidal capillary has been used at different synchrotron sources.[4,5] However, because of the special shape of the ellipsoidal capillary, to make an ellipsoidal capillary with good quality is a great challenge. The quality of an ellipsoidal capillary is mainly quantified by the transmission efficiency, the full width at half maximum (FWHM) of the focused beams and the power density gain of the device. In order to improve its quality, mathematic model and computer simulation methods are very important.

In this paper, using a ray-tracing method, we develop a computer simulation program to study the transmission function of ellipsoidal capillary, and analyse quantitatively the influence of the parameters of ellipsoidal capillary on the quality of the ellipsoidal capillary by using this program.

2. Simulation model

In recent decades, researchers have developed several methods to calculate different capillaries transmission function.[6−13] Gibson group used pseudo-gravitational acceleration model to simulate x-ray transmission through a cylindrical bending capillary, and obtained an approximate result.[6] Furuta and Vincze groups used a ray-tracing method to get the images of x-rays after tapered mono-capillary.[8,9] Liu used SHADOW program to calculate x-ray transmission in tapered mono-capillary and polycapllary x-ray lens.[11−13] In 2001, Bilderback and Huang used a geometrical optics method to simulate the focal spot size and intensity gain from an ellipsoidal one-bounce glass mono-capillary.[14] This method can only record the one-bounce x-rays through an ellipsoidal capillary and neglect the second-bounce x-rays. The second-bounce x-rays are very small and are not expected, but they are existent.[4]

In this paper, we use a ray-tracing method[15,16] to simulate the propagations of x-rays through an ellipsoidal capillary. This method can trace all x-rays through the capillary.

Figure 1 shows the schematic diagram of x-ray transmission in an ellipsoidal capillary. The broken curve shows an ellipsoid. We can see that an ellipsoidal capillary is the ring-shaped section of an ellip-

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soid. The spots o and o_1 are the two focal points of the ellipsoid. The x-ray source is located at spot o and x-rays emitted from the source can be focused at spot o_1. The D is the distance between the x-ray source and the entrance of ellipsoidal capillary, L is the length of ellipsoidal capillary and f is the distance between the exit of ellipsoidal capillary and the second focus. The relationship between D, L and f can be expressed as

$$D + L + f = 2c, \tag{1}$$

where $2c$ is the distance between the two focal points.

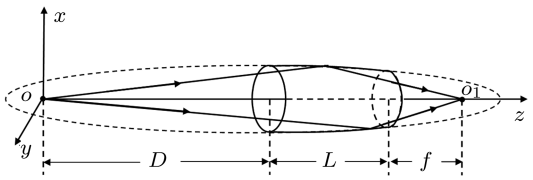


Fig. 1. The schematic diagram of x-rays transmission in an ellipsoidal capillary.

The profile of an ellipsoidal capillary can be expressed as:

$$\frac{x^2}{a^2} + \frac{y^2}{a^2} + \frac{(z - z_0)^2}{b^2} = 1, \quad D \le z \le D + L, \tag{2}$$

where a and b are the semi-minor axis and the semi-major axis of the ellipsoid, respectively, (0, 0, z_0) is the coordinate of the centre of the ellipsoid. In our previous works, the ray-tracing method has been introduced in details.[17,18] The external normal of the wall of the ellipsoidal capillary $\boldsymbol{n}$ can be expressed as

$$\boldsymbol{n} = (n_x, n_y, n_z) = \left(\frac{\frac{x}{a^2}, \frac{y}{a^2}, \frac{z - z_0}{b^2}}{\sqrt{\frac{x^2}{a^4} + \frac{y^2}{a^4} + \frac{(z - z_0)^2}{b^4}}} \right). \tag{3}$$

The direction cosine of x-rays emitted from source is

$$\begin{aligned} \boldsymbol{\mu}_i &= (\mu_x, \mu_y, \mu_z) \\ &= \frac{(x_\mathrm{p} - x_\mathrm{s}, y_\mathrm{p} - y_\mathrm{s}, z_\mathrm{p} - z_\mathrm{s})}{\sqrt{(x_\mathrm{p} - x_\mathrm{s})^2 + (y_\mathrm{p} - y_\mathrm{s})^2 + (z_\mathrm{p} - z_\mathrm{s})^2}}, \end{aligned} \tag{4}$$

where $(x_\mathrm{s}, y_\mathrm{s}, z_\mathrm{s})$ is the coordinate of a point on the extended x-ray source and $(x_\mathrm{p}, y_\mathrm{p}, z_\mathrm{p})$ is the coordinate of a point on the entrance of ellipsoidal capillary.

According to the ray-tracing method, the glancing incident angle θ and the reflected vector $\boldsymbol{\mu}_r$ can be expressed as

$$\theta = \arcsin(\boldsymbol{n} \cdot \boldsymbol{\mu}_i), \tag{5}$$

$$\boldsymbol{\mu}_r = \boldsymbol{\mu}_i - 2\boldsymbol{n} \sin\theta. \tag{6}$$

With these equations, all photons' paths can be traced and all the coordinates at the receiving screen of the photons exiting from the ellipsoidal capillary can be recorded. According to these coordinates at the receiving screen, we can use two methods to express the intensity distribution, three-dimensional (3D) image (X–Y–I) and two-dimensional (2D) image (X–I). The 2D image is Gauss-curve and the FWHM can be calculated.

The transmission efficiency (η) of x-ray beams through a capillary is defined as

$$\eta = I_\mathrm{out}/I_\mathrm{in}, \tag{7}$$

where I_out is the flux of x-ray beams departing from the exit and I_in is the flux of x-ray beams entering the capillary. In simulation mode, all incident x-rays are controlled by the source and the entrance of capillary. The flux of exit beams includes pass-through beams and reflected beams, we use numerical integration to calculate I_out and I_in.

The power density gain (G) of capillary is defined as the ratio of the x-ray flux with and without capillary, and is expressed as

$$G = I_\mathrm{with}/I_\mathrm{without}, \tag{8}$$

where I_with and I_without describe the x-ray flux with and without capillary, respectively. Generally, we choose a receiving pinhole, the diameter is equal to the FWHM of the x-ray beams exiting from the capillary, to calculate the power density gain.

3. Simulation results and discussion

In the following results, the radius of extended sources is 0.025 mm, and the source is put on the first focus. The main material of ellipsoidal capillary is borosilicate. The density of the material is 2.2 g/cm^2.

3.1. Intensity distribution

In this program, we use 2D plane image and 3D image to show the focused x-rays intensity distribution. Figures 2 and 3 exhibit these images. The parameters of the ellipsoidal capillary are: the semi-minor axis a = 0.5 mm, the semi-major axis b = 250 mm, and the distance between the x-ray source and the entrance of capillary D = 300 mm. The energy of the simulated x-ray source is 8.04 keV. Figure 2 shows the simulated 2D and 3D images at f = 5 mm. The position at f = 5 mm is the second focus of the

ellipsoidal capillary. We can see that most x-rays are focused at the second focus, and the FWHM of x-ray beams is about 16 μm. Compared with the intensity of the central x-ray, the marginal pass-through x-ray intensity is much fainter, and the ratio of the power density is about thousandfold. Figure 3 shows the simulated 2D and 3D images at the position which is 495 mm away from the second focus along the semi-major axis. The central dark spot is the pinhole image of the x-ray source, and the dark ring is the reflected x-ray beams. This image is similar to the experimental result in Ref. [4].

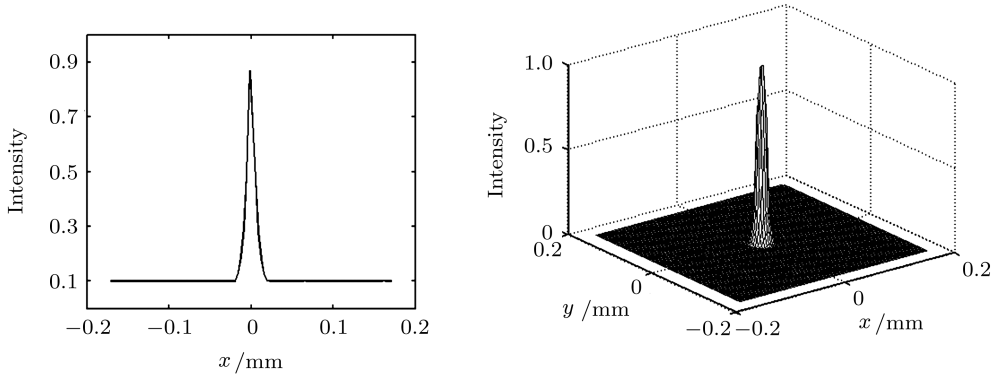


Fig. 2. The 2D and 3D images after the ellipsoidal capillary at the second focus ($f = 5$ mm).

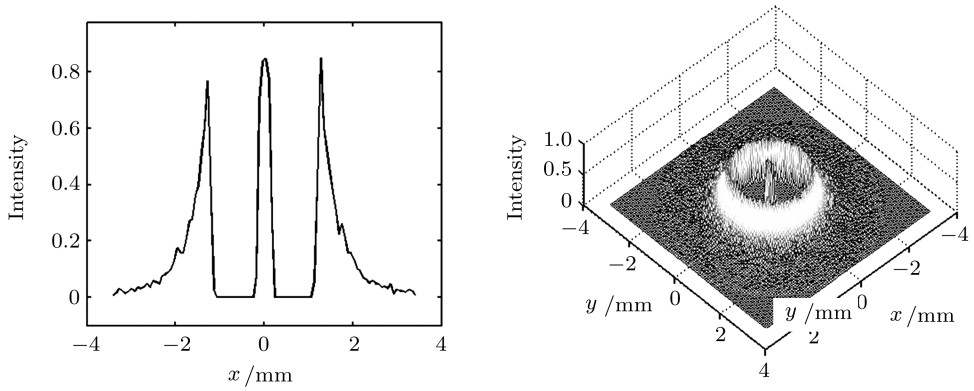


Fig. 3. The 2D and 3D images after the ellipsoidal capillary at the position which is 495 mm away from the second focus along the semi-major axis ($f = 500$ mm).

3.2. Simulated η, gain and FWHM

3.2.1. Length of ellipsoidal capillary

The length (L) of ellipsoidal capillary is one of the important parameters. From Fig. 1 and Eq. (2), we can see when the parameters a, b, c and f of the ellipsoidal capillary are fixed, with the increase of the D, the length L of the capillary decreases. Figure 4 shows the influence of the length of ellipsoidal capillary on the η, gain and FWHM. The simulated ellipsoidal capillary are: the semi-minor axis $a = 0.5$ mm, the semi-major axis $b = 150$ mm, and $f = 5$ mm. The energy of the simulated x-rays is 8.04 keV.

From Fig. 4 we can see that with the increase of L, the transmission efficiency curve ascends first, and then descends. Coincidentally, the FWHM and the power density gain increase with the increase of L. With $L > 215$ mm, the transmission efficiency curve descends and the FWHM and the power are almost invariable. This is caused by the small critical angle. With the increase of L, when the angle of incidence is bigger than the critical angle, although the receiving solid angle is bigger, the incremental x-rays can not be reflected. For a high-quality ellipsoidal capillary, the higher η, the larger gain and the smaller FWHM are expected. So we should take into account the experimental request to use longer L to get a larger gain or use shorter L to get smaller FWHM. We can also choose an appropriate length to get suited gain and FWHM fulfilling the experimental request.

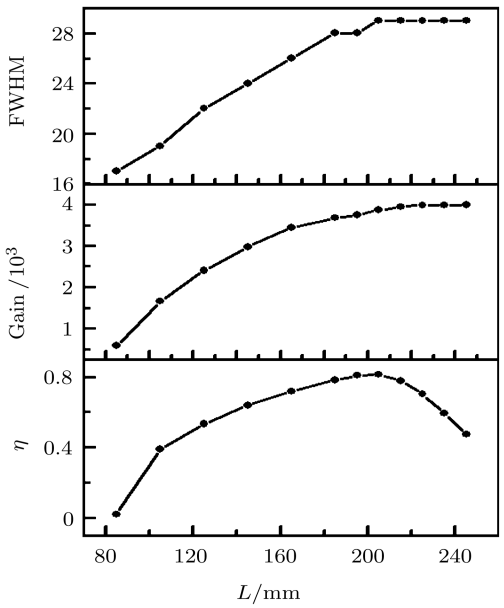


Fig. 4. The influence of L on the η, gain and FWHM.

3.2.2. Different part of the ellipsoidal capillary

For an ellipsoidal capillary, the FWHM, in other words, the image size is decided by the part of the ellipsoidal capillary reflecting x-rays. Table 1 shows the FHWM with different part of the ellipsoidal capillary.

Table 1. The FHWM with different part of the ellipsoidal capillary.

D/mm	f/mm	FWHM/mm
95	355	0.150
145	305	0.090
195	255	0.055
245	205	0.036
295	155	0.028
345	105	0.016
395	55	0.015

In order to choose different part of the ellipsoidal capillary to transmit x-rays, we first fix the length of the ellipsoidal capillary $L = 50$ mm, and then change the value of D. According to the Eq. (1) in Section 2, the value of f will be larger with smaller D. The smaller the value of D is, the more anterior the reflecting surface is. From Table 1, we can see that if the reflecting surface is the anterior part of the ellipsoidal capillary, the FWHM is larger, on the contrary, if the reflecting surface is the tail part of the ellipsoidal capillary, the FWHM is smaller. Equation (1) in Ref. [14] can also show this rule. It is useful for explaining the conclusion in the next section. The parameters of the ellipsoidal capillary are: $a = 0.35$ mm, $b = 250$ mm, and the energy of the simulated x-ray source is 10 keV.

3.2.3. The x-ray energy

For different x-ray energy, the glass capillary has a different index of reflection and absorption and the critical angle of total reflection. The higher the energy is, the smaller the critical angle is. Figure 5 shows the influence of x-ray energy on the η, gain and FWHM. With the increase of x-ray energy, the

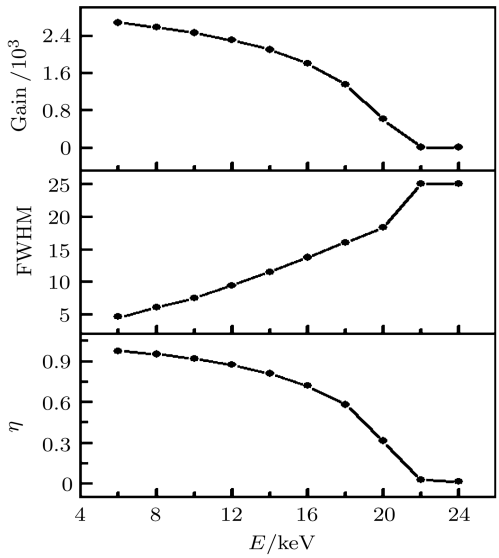


Fig. 5. The influence of E on the gain, FWHM and η.

η of the ellipsoidal capillary decreases, the same as the character of polycapillary x-ray lens.[19] At the same time, we found a special conclusion different from polycapillary x-ray lens and tapered capillary, the FWHM of the ellipsoidal capillary becomes larger with higher energy.[19] For high energy x-rays, because of the smaller critical angle, the x-rays hitting at the tail part of the ellipsoidal capillary can not be reflected, in other words, the reflecting surface is the anterior part of the ellipsoidal capillary. So according to the conclusion in Section 2, the FWHM of high energy x-rays is larger than low energy x-rays. Accordingly, with smaller η and larger FWHM, the gain decreases with the increase of x-ray energy. We can see that when x-ray energy E increases to 22 keV, only pass-through x-rays can be detected, therefore, the η is close to zero.

3.2.4. Distances from two focal points

According to the schematic diagram Fig. 1, we know that in order to fully exert the function of the ellipsoidal capillary, the x-ray source and the detection position should be put on the two focal points of the ellipsoidal capillary. In Fig. 6 the x-axis shows the

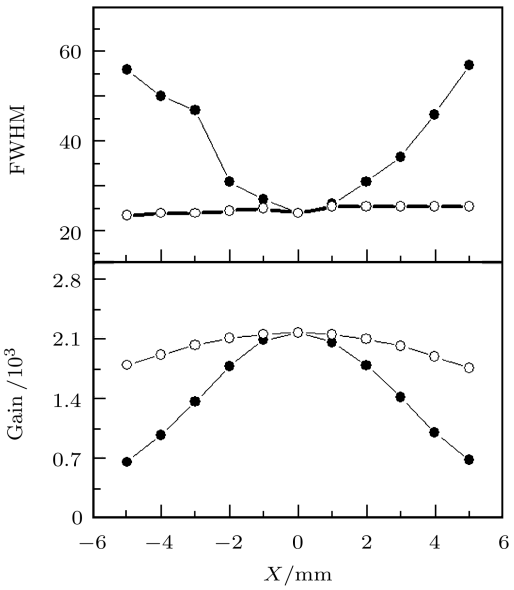


Fig. 6. The influences of the distances away from two focal points on the FWHM and gain: open circle for the curve of distance away from the first focal point; point circle for the curve of distance away from the second focal point.

distances from two focal points along the semi-major axis of the ellipsoidal capillary, and the position at $x = 0$ is the focus of the ellipsoidal capillary. We can see that the position of x-ray source has little influence on the FWHM and gain, and the distance from the second focal point has large influence. This is because for this ellipsoidal capillary: $D = 150$ mm and $f = 5$ mm. $f \ll D$ causes this result.

4. Conclusion

Using the ray-tracing method, we can trace the propagations of x-rays through ellipsoidal capillary. According to the above simulated results, the conclusions have reached: 1) the transmission efficiency, the FWHM and the power density gain are greatly affected by the parameters of ellipsoidal capillary; 2) the FWHM and the power density gain are different from polycapillary x-ray lens, the FWHM of ellipsoidal capillary becomes larger with higher energy. With this simulation program, we can also design the parameters of the ellipsoidal capillary based on experimental requirements.

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