A simulation model and experimental study of X-ray transmission through a polycapillary focusing X-ray lens

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Abstract. A simulation model is established to simulate the X-ray transmission performance through a polycapillary focusing X-ray lens whose configuration curve was described by a piecewise function. The shape of the lens is segmented, and each segment uses different function curve. The ray tracing principle is used to simulate the transmission performance of X-rays through the polycapillary focusing X-ray lens. And the simulation results were compared with the experimental results.

1. Introduction
Micro-X-ray analyse as the non-destructive analytical tools, has been widely used in many fields such as materials science, environmental science, archaeology and life sciences [1-4]. Polycapillary X-ray lenses can effectively guide wide-band X-rays based on the total reflection principle [5-6]. According to its function, polycapillary X-ray lenses can be divided into two major categories: polycapillary parallel X-ray lens and polycapillary focusing X-ray lens. Polycapillary parallel X-ray lenses can efficiently collect divergent X-rays to form quasi-parallel X-ray beams [7-9]. Polycapillary focusing X-ray lenses can focus X-rays to a micro-scale focal point, thereby obtaining high power density gain [10], which has been widely applied in X-ray fluorescence analysis and X-ray imaging. In order to predict the transmission performance of the polycapillary X-ray lens, plenty of simulation programs have developed [11-14]. For a polycapillary focusing X-ray lens, the center line of each single capillary is usually described by a specific equation. In Takano’s model, the entire external shape of the polycapillary optics was described by a part of the function f(z). In Liu’s model and Peng’s model, the shape of the polycapillary focusing X-ray lens was described by part of a quadratic curve equation. Hampai’s model uses an elliptical toroid to express the shape of the full lens, and each channel axis describes as a part of an ellipse. However, in practical application, due to the need of experiment and the limitation of manufacturing technology, the shape of polycapillary focusing X-ray lenses usually cannot be expressed exactly by one function. In addition, the shape of the lens is one of the most important factors affecting transmission performance. In this paper, the shape of the polycapillary focusing X-ray lens is described by a segment function, with the maximum radius of the lens as the dividing point, and the two segments are described with different quadratic curves. The transmission performance of the lens was calculated, and the simulation results were compared with the experimental results, which proved that the experimental results were in good agreement with the simulation results.

2. Simulation model
A simulation program was compiled with MATLAB. In this simulation model, the configuration curve of the polycapillary focusing X-ray lens is divided into two parts, which were represented by quadratic functions \( f_1(z) \) and \( f_2(z') \), respectively. As shown in Figure 1, the highest point of the polycapillary focusing X-ray lens serves as the boundary between parts 1 and 2. \( L \) is the length of the polycapillary focusing X-ray lens, \( L_1 \) and \( L_2 \) are the length of the part 1 and part 2, respectively. The inlet radius, outlet radius and maximum radius of the polycapillary focusing X-ray lens are \( R_{in} \), \( R_{out} \), and \( R_{max} \), respectively.

2.1. Geometry model of the polycapillary focusing X-ray lens

Polycapillary focusing X-ray lens consists of hundreds of thousands of single capillaries, the capillaries are arranged in a hexagonal structure and symmetrically around a centerline. To simulate the transmission performance of the polycapillary focusing X-ray lens, it is necessary to calculate the inner wall equation of the single capillary. First, we calculate the central coordinates of each capillary at the
entry of the polycapillary focusing X-ray lens. As shown in figure 2, the capillaries are divided into six regions. In region 1, the center coordinates of the capillary i on layer k are \((x_{ki}, y_{ki})\).

\[ x_{ki} = (2k - i - 1)d_x \]
\[ y_{ki} = (i-1)d_y \]

(1)  (2)

where \(d_x\) and \(d_y\) can be expressed as

\[ dx = r_{in} \]
\[ dy = \sqrt{3}r_{in} \]

(3)  (4)

where \(r_{in}\) is the capillary radius at the entrance of the lens. The coordinates of other regions are obtained by coordinate rotation. The configuration curve of the polycapillary focusing X-ray lens in part 1 is represented by \(f_1(z)\). In the \(\theta-xyz\) coordinate, \(f_1(z)\) can be expressed as \(f_1(z) = a_1z^2 + a_2z + a_3\).

The centerline of the capillary in part 1 can be expressed as

\[ X_{ki}(z) = x_{ki} f_1(z) / R_m \]
\[ Y_{ki}(z) = y_{ki} f_1(z) / R_m \]

(5)  (6)

The capillary radius changes with the length of the polycapillary focusing X-ray lens, which can be expressed as

\[ r(z) = r_{in} f_1(z) / R_m \]

(7)

Therefore, the profile of capillary’s inner wall in part 1 can be expressed as \(F_1(x, y, z) = 0\).

\[ F_1(x, y, z) = \left[ x - X_{ki}(z) \right]^2 + \left[ y - Y_{ki}(z) \right]^2 = \left[ r(z) \right]^2 \]

(8)

In part 2, under \(\phi'-x'y'z'\) coordinate, \(f_2(z')\) can be expressed as \(f_2(z') = b_1z'^2 + b_2z' + b_3\). In this part, the centerline of the capillary i on the layer k can be expressed as

\[ X_{ki}'(z') = x_{ki} f_1(L_i) f_2(z') / R_m R_{max} \]
\[ Y_{ki}'(z') = y_{ki} f_1(L_i) f_2(z') / R_m R_{max} \]

(9)  (10)

And the radius of the capillary in part 2 can be expressed as

\[ r'(z') = r_{ki} f_1(L_i) f_2(z') / R_m R_{max} \]

(11)

The profile of capillary’s inner wall in part 2 can be expressed as \(F_2(x, y, z) = 0\).

\[ F_2(x', y', z') = \left[ x' - X_{ki}'(z') \right]^2 + \left[ y' - Y_{ki}'(z') \right]^2 = \left[ r'(z') \right]^2 \]

(12)

2.2. Transmission of X-rays through the polycapillary focusing X-ray lens
As mentioned above, polycapillary focusing X-ray lens is an array of single capillaries. Therefore, we need to calculate the transmission of X-rays in single capillary channel. In this model, the X-rays transmit through the single capillary channel contains two parts. As shown in Figure 3, D is the distance between the entrance of the capillary channels and the X-ray source. $L_1$ and $L_2$ are the length of the part 1 and part 2, respectively. $S(x_s, y_s, z_s)$ refers to coordinates of the X-ray source, and $P(x_p, y_p, z_p)$ is a point on the entrance of a single capillary channel. The unit vector of incident X-ray can be expressed as

$$\vec{u} = (u_x, u_y, u_z) = \left( x_p - x_s, y_p - y_s, z_p - z_s \right) \left[ (x_p - x_s)^2 + (y_p - y_s)^2 + (z_p - z_s)^2 \right]^{-1/2}$$

(13)

The intersection point of incident X-ray and capillary inner wall can be obtained by using the iterative method. In addition, at the intersection point, the external unit vector of the capillary’s inner wall is

$$\vec{n} = (n_x, n_y, n_z) = \left( N_x, N_y, N_z \right) \left[ (N_x)^2 + (N_y)^2 + (N_z)^2 \right]^{1/2},$$

(14)

where

$$N_x = \frac{\partial F_1(x, y, z)}{\partial x}$$

$$N_y = \frac{\partial F_1(x, y, z)}{\partial y}$$

$$N_z = \frac{\partial F_1(x, y, z)}{\partial z}$$

If the intersection is in the first part of the capillary, according to the ray-tracing principle, glancing angle $\theta$ and the reflected direction $r$ can be determined by

$$\theta = \sin^{-1} \left( \vec{u} \cdot \vec{n} \right)$$

(15)

$$r = \vec{u} - 2\vec{n} \sin \theta$$

(16)

If the glancing angle $\theta$ is less than or equal to the critical angle, we consider its reflected X-rays as the incident X-rays until the X-rays departing from the part 1 of the capillary. Suppose the unit vector of the X-ray emission direction is $\vec{u}_n$. Then, we consider the X-ray departing from the part 1 of the capillary as the incident X-ray. Under $o' - x'y'z'$ coordinates, the unit vector of incident X-ray can be expressed as

**Figure 3.** Schematic of X-ray transmission through a single capillary.
Similarly, ray tracing is used to track the X-ray transmission through the part 2. Suppose the unit vector in the direction of the X-ray departing from the part 2 is \( \mathbf{u} \), and the last reflection point is \( (x_n', y_n', z_n') \). The coordinates of the photon at observation plane can be expressed as

\[
\begin{align*}
x_f &= x_n' + \frac{u_{nx}}{u_{nz}} (L_2 + f - z_n') \\
y_f &= y_n' + \frac{u_{ny}}{u_{nz}} (L_2 + f - z_n')
\end{align*}
\]

where \( f \) represents the distance from the exit of the polycapillary focusing X-ray lens to the observation panel. As is known to all that the polycapillary focusing X-ray lens composed an array of single capillaries. Then it is easy to calculate all the coordinates of the photons emitted from the lens.

2.3. Calculation of the transmission efficiency of the polycapillary focusing X-ray lens.

In this simulation model, we consider the entrance of the lens is divided into \( N_1 \) parts, so the flux of X-ray beams entering the polycapillary focusing X-ray lens can be expressed as

\[
I_{in} = N_1
\]

The flux of X-ray beams emitted from the exit of the lens contains of the reflected beams and the pass-through beams, which can expressed as

\[
I_{out} = \sum_{n_1} n_1 + \sum_{n_2} [1 \times \prod_{M,M'} (R_{\phi})_{m}]
\]

where \( n_1 \) and \( n_2 \) indicate the number of the pass-through and reflected X-ray beams, respectively; \( (R_{\phi})_{m} \) is the reflectivity of X-ray at the \( m \)th reflection; \( M \) and \( M' \) represent the reflection number in the part 1 and part 2, respectively. The transmission efficiency of X-rays through a polycapillary X-ray lens can defined as

\[
\eta = \frac{I_{out}}{I_{in}}
\]

3. Results and discussion

To verify the validity of the simulation program, an experimental setup, as shown in figure 4, was built in the X-ray Lab of BNU. The X-ray source was provided by a Cu anode X-ray generator, which was produced by the Trufocus company in the United States. The focal spot of the X-ray source is 8 μm. In this experiment, the operating voltage and current were 25 kV and 0.15 mA, respectively. The entrance of the polycapillary focusing X-ray lens was placed at a distance of 120 mm from the X-ray source. A lead sheath was used to shield stray light. The parameters of the polycapillary focusing X-ray lens were as follows: The inlet and outlet radius of the lens were 2.64 and 2.13 mm, respectively. The length of the part 1 and part 2 were 15.5 and 19.5 mm, respectively. The polycapillary focusing X-ray lens was adjusted by a five-dimensional adjusting frame whose rotational and translational adjustment accuracy are 0.003 deg and 2μm, respectively. The five-dimensional adjusting frame is produced by SURUGA SEIKI Co., Ltd. As mentioned above, the transmission efficiency (\( \eta \)) is defined as \( \eta = \frac{I_{out}}{I_{in}} \). In the experiment, \( I_{out} \) is the flux of the X-ray beams departing from the polycapillary focusing X-ray lens, whose value is recorded by an X-ray detector placed behind the exit of the polycapillary focusing X-ray lens.
lens. $I_{in}$ is the flux of X-ray beams that enter the polycapillary focusing X-ray lens. To obtain its value, polycapillary focusing X-ray lens needs to be replaced by a diaphragm with a diameter of 3 mm, and the diaphragm was 120 mm from the X-ray source. X-rays that transmit through the diaphragm are received and recorded by the detector. In this step, to ensure that the emitted X-rays are received by the detector, the detector should be close to the diaphragm. Under above experimental conditions, the measured transmission efficiency was 31%, which is lower than the simulation results 49%. This is because the simulation conditions are ideal conditions, and the lens actually produced has defects due to production process limitations. Moreover, the inner wall of the actual lens is not completely smooth, which is also one of the main causes of the difference.

![Figure 4. Schematic configuration of the experiment device. (PFXL represent the polycapillary focusing X-ray lens).](image)

In addition, the focal length and focal spot size of the polycapillary focusing X-ray lens were obtained by the knife-edge scanning method [10], the knife-edge scanning was performed at different distance to the exit of the lens, and the step size was 20 μm. In this way, the integral curves of the X-ray intensity distributions at different positions were measured. Then the integral curve was differentiated, the FWHM of the Gaussian fit of the differential curve was the beam spot size at that position. The experimental results show that the smallest spot size is 86 μm at 28 mm from the exit of the polycapillary focusing X-ray lens. Figure 5 shows the differential curve of the X-ray intensity distribution at the focal spot of the polycapillary X-ray lens. The simulation results of the focal length and focal spots are 28 mm and 78 μm, respectively. The experimental results are basically consistent with the simulation results.
4. Conclusion
A simulation model is established to simulate the X-ray transmission performance through polycapillary focusing X-ray lens whose configuration curve was described by a piecewise function. Compared with the polycapillary X-ray lens whose configuration curve is described by the same function, this model allows for more flexible drawing of the shape of the polycapillary X-ray lens to meet different experimental needs. Through optimizing the profile curve of the first part of the polycapillary focusing X-ray lens, more X-rays that satisfy the total reflection condition can enter the lens. Then, through optimizing the profile curve of the first part of the polycapillary focusing X-ray lens, the X-ray beams are effectively converged to obtain a smaller focal spot or a smaller divergence. With this simulation program, we can design the parameters of the polycapillary focusing X-ray lens to the experimental requirements.

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