Polycapillary X-ray lens for the secondary focusing Beijing synchrotron radiation source*

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According to intensity distribution of the synchrotron radiation source focused by a toroidal mirror at the Beijing synchrotron radiation biological macromolecule station, theoretical modeling of the Beijing synchrotron radiation source is developed for capillary optics. Using this theoretical modeling, the influences of the configuration curve of the polycapillary X-ray lens on transmission efficiency and working distance are analyzed. The experimental results of the transmission efficiency and working distance at the biological macromolecule station are in good agreement with the theoretical results.

Keywords: Beijing synchrotron radiation facility, polycapillary X-ray lens, secondary focusing

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1. Introduction

A synchrotron radiation source with high brightness, good collimation, and continuous energy distribution is an important tool for revealing the material structure and phenomenon of life, and is widely used in materials, geological, biological, environmental, and archaeological fields, and so on. With the development of synchrotron radiation technology, the X-ray microbeam analysis technique using focusing optical devices is becoming an important method.[1–3]

The Beijing synchrotron radiation facility (BSRF) is a first-generation Synchrotron Radiation Source, so the spot size and divergence are rather large. In order to obtain a microfocus X-ray beam, a slit is usually used to restrict the incoming X-ray beam in the BSRF, and only part of the total luminous flux can be used. So for obtaining more flux and increasing X-ray beam intensity, X-ray focusing optics are required to perform the secondary focus of the X-ray beam.

At present, there are some X-ray focusing optical elements, such as a KB mirror, compound refractive lens, Fresnel zone plates, and multilayer Laue lens. These devices each have the advantage of a small focal spot (as small as the dozens of nm available currently), but at the same time they have different problems, such as narrow energy ranges, small acceptance angles, etc. In addition, to effectively achieve focus, these X-ray focusing optical elements each need a large object/image ratio. Based on the X-ray total reflection principle, polycapillary X-ray optics has a wide energy range and an acceptance angle. Polycapillary X-ray optics is not an imaging optical element, and X-ray source fluctuation and instability affect neither the focal spot position nor size. Because of the appearance of axial symmetry, the thermal gradient does not affect the focal spot position. When the optical system is only used to focus an X-ray beam, the non-imaging optical element is superior to the imaging optical element.[4] So polycapillary X-ray optics is an ideal secondary focusing optical element on the BSRF.

2. Theoretical simulation of the primary focusing source of Beijing synchrotron radiation

2.1. Intensity distribution of the primary focusing source

The Beijing synchrotron radiation biological macromolecule station (1W2B) includes a collimating mirror, a double-crystal monochromator, and a toroidal mirror. The X-ray energy used for the biological macromolecular diffraction experiment is 12.4 keV. The length of the toroidal mirror is 1 m, and the distance between the center of the mirror and the focusing spot is 9.54 m. The size of the X-ray beam focused by the double-crystal monochromator is 40.5 mm(H)×3.5 mm(V), the X-ray beam is focused by a toroidal mirror to 0.9 mm(H)×0.6 mm(V), and the divergence is about 1.7 mrad(H)×0.17 mrad(V).

Using a conventional metal knife edge scanning method, we measure the primary focusing spot intensity distribution. Figure 1 shows the differential and integral curves of the primary focusing spot along the horizontal direction. The full width at half maximum (FWHM) of the differential curve is 0.86 mm. Along the beam transmission direction, the size of the focusing beam is still about 0.86 mm at a distance of

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200 mm. The distance is the so-called 'focal depth'.

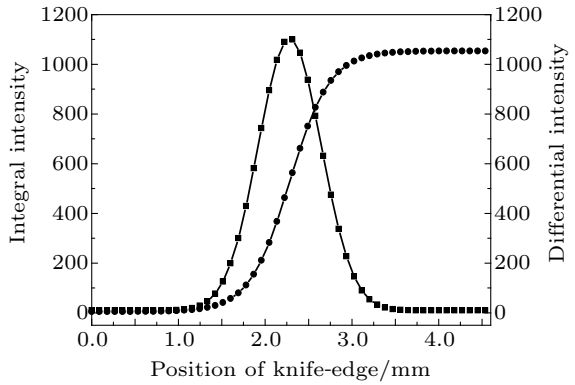


Fig. 1. The differential curve and the integral curve in a horizontal direction.

2.2. Theoretical modeling of the primary focusing source

According to the above experimental results, the X-ray beam focused by the toroidal mirror is shown in Fig. 2. At the end of the 'focal depth', the X-ray beam is divergent, and has a Gaussian-like distribution. Because of these features, the polycapillary X-ray lens is very adaptive to the secondary focusing device. The polycapillary X-ray lens can be located at a distance away from the end of the 'focal depth', and the distance is f_1, as shown in Fig. 2. The polycapillary X-ray lens will have a high transmission efficiency for the primary focusing source.

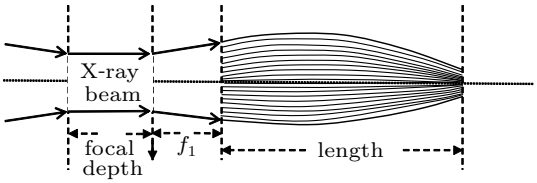


Fig. 2. Schematic diagram of the polycapillary X-ray lens used in the primary focusing source.

In contrast to the laboratory X-ray source,[5,6] the primary focusing source can be simulated as a divergent and Gaussian-like distribution source. In the MATLAB program, we use the 'normrnd' function to describe the Gaussian distribution of the X-ray beam intensity, and it is expressed as

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right], \tag{1}$$

where μ and σ are the mean value and variance of the Gaussian function, respectively.

The FWHM of the X-ray beam intensity can be expressed as

$$\text{FWHM} = 2\sqrt{2\ln 2}\sigma \approx 2.3548\sigma. \tag{2}$$

By setting the value of σ, we can simulate the same FWHM with the experimental value at the 1W2B station. Then, the simulated Gaussian distribution source emits X-ray beams that have the same divergence as the experimental X-ray beams.

In order to verify the correctness of the theoretical modeling of the primary focusing source, the theoretical results are compared with the experimental results. Figure 3 shows the ratios of X-ray intensity with different circular apertures in the 'focal depth' region. The ratio is calculated by I/I_0, where I_0 is the total intensity of the primary focusing source and I is the X-ray intensity inside the circular aperture. An open circle curve represents the experimental results of the real X-ray source and a solid circle curve denotes the theoretical results. We can see that the theoretical results are in good agreement with the experimental results.

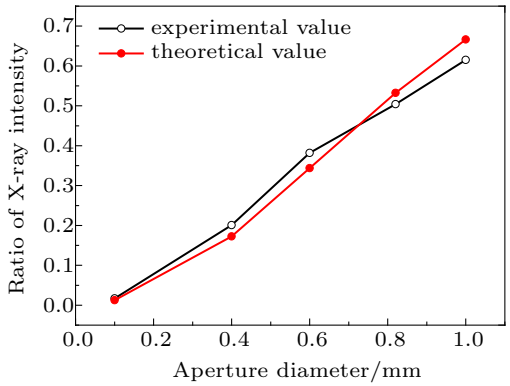


Fig. 3. Ratios of X-ray intensity with different circular apertures.

Table 1 shows the FWHM values of the X-ray beam at different distances from the end of the 'focal depth'. At the end of the 'focal depth', the X-ray beam is divergent and we use the same divergence in theoretical modeling with a real X-ray beam with a size of 1.6 mrad(H)×0.17 mrad(V). We can therefore see that the theoretical results are close to the experimental results.

Table 1. The diameters of the focusing spots at different distances from the exit of the focal depth.

Distance from the exit of focal depth/ mm	0	20	30	50	70
Experimental results/μm	869	882	902	933	966
Theoretical results/μm	860	895	908	939	973
Deviation	1.0%	1.5%	0.7%	0.6%	0.7%

In short, through the comparison between the experimental and theoretical results, we can find that the experimental and theoretical results are in agreement very well, which means that the theoretical modeling of the primary focusing source reflects the real intensity distribution at the 1W2B station. The theoretical modeling can also be used for other Beijing synchrotron macromolecule stations.

3. Theoretical calculation of the transmission properties of the polycapillary X-ray lens

3.1. Simulation model of the polycapillary X-ray lens

In recent decades, researchers have developed several methods to calculate different capillary transmission

functions.[7–14] In the present paper, we use the ray-tracing method to simulate the propagations of X-rays through a polycapillary X-ray lens. This method can trace all X-rays through each capillary.

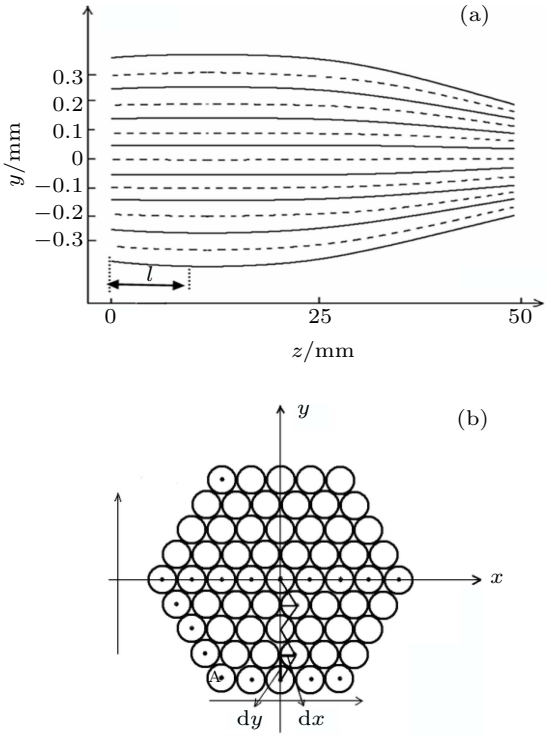


Fig. 4. Schematic diagram of a polycapillary X-ray lens, showing the axial (a) and transverse (b) cross section.

A polycapillary X-ray lens is composed of 100,000 curved glass capillaries. Its cross section is regular hexagonal. Figure 4 is a schematic diagram of the polycapillary X-ray lens. Two functions are needed to describe the spatial equation of each capillary. One function, $g(z)$, is used to represent the central axis equation of every capillary, and the other function, $f(z)$, is used to represent the radius change equation of each capillary with a z axis. Based on the shape of the polycapillary X-ray lens, $g(z)$ and $f(z)$ can be expressed as quadratic functions as follows:

$$g(z) = A_1 \cdot z^2 + A_2 \cdot z + A_3, \tag{3}$$

$$f(z) = B_1 \cdot z^2 + B_2 \cdot z + B_3, \tag{4}$$

where A_1, A_2, A_3, B_1, B_2, and B_3 are the function coefficients, and they can be calculated as

$$A_1 = B_1 = (r_{\text{in}} - r_{\text{max}})/(r_{\text{in}} \cdot l^2), \tag{5}$$

$$A_2 = B_2 = -2A_1 \cdot l, \tag{6}$$

where r_{in} is the entrance radius of a capillary, r_{max} the maximum radius of a capillary, and $|l|$ the distance between the entrance and the maximum radium position.

Let $A_3 = B_3 = 1$, then the center coordinates of each capillary in the entrance end of the X-ray lens will be conveniently described.

Because of the relationship between r and R:

$$\frac{r_{\text{in}}}{R_{\text{in}}} = \frac{r_{\text{out}}}{R_{\text{out}}} = \frac{r_{\text{max}}}{R_{\text{max}}}, \tag{7}$$

where r is the radius of a capillary and R the radius of a polycapillary X-ray lens, and the coefficients of two functions, $g(z)$ and $f(z)$, can be calculated with R_{in} and R_{max}.

The spatial equation of each capillary can be expressed as

$$[X - X_0(k) \cdot g(z)]^2 + [Y - Y_0(k) \cdot g(z)]^2 = [r_{in} \cdot f(z)]^2, \tag{8}$$

where $(X_0(k) \cdot g(z), Y_0(k) \cdot g(z))$ is the center coordinate of each capillary on the x–o–y plane that is located at the entrance of the polycapillary, and its value is determined by the location of the capillary.

The transmission efficiency (η) of the X-ray lens is defined as $\eta = I_{\text{out}}/I_{\text{in}}$, where I_{out} is the flux of the X-ray beams departing from the exit, and I_{in} the flux of X-ray beams entering the capillary. Using the ray-tracing method,[5] we can trace all X-rays to obtain I_{in} and I_{out}. So we can calculate the transmission efficiency (η) of the polycapillary X-ray lens.

Using the theoretical model of the primary focusing source and polycapillary X-ray lens, we calculate the transmission efficiencies of the polycapillary X-ray lens with different values of l. The parameters of the simulated X-ray source are as follows: the geometric size is 0.86 mm(H)×0.53 mm(V), and the divergent size is 1.6 mrad(H)×0.17 mrad(V). The parameters of the X-ray lens are as follows: length = 40 mm, entrance radius $r_{\text{in}} = 5$ μm , exit radius $r_{\text{out}} = 3$ μm, and X-ray energy $E = 12.4$ keV. Table 2 shows the values of the transmission efficiency η of the polycapillary X-ray lens with different values of l. From Fig. 2, we know that the z-axis coordinate of the entrance of the polycapillary X-ray lens is zero, and l is the z-axis coordinate of the maximum radium position of the polycapillary X-ray lens. When $l > 0$, the maximum radium position is on the left of the entrance of the polycapillary X-ray lens; when $l < 0$, the maximum radium position is on the right of the entrance; and when $l = 0$, the maximum radium position is the entrance of the polycapillary X-ray lens. When $l = 1.8$ mm, the transmission efficiency η of the polycapillary X-ray lens reaches the maximum value 52.5%.

Table 2. The transmission efficiencies of the polycapillary X-ray lens with different values of l.

l/mm	−1.5	0	1.5	1.8	2.0	2.5
η	47.8%	50.7%	52.0%	52.5%	52.4%	52.3%

Using the same method as that in Table 2, we can obtain the best value of l with the maximum transmission efficiency. Table 3 shows the calculation results with different polycapillary X-ray lenses. The other parameters of the X-ray lens are as follows: the length of the X-ray lens is 40 mm, the entrance radius $r_{\text{in}} = 5$ μm, and the X-ray energy $E = 12.4$ keV. We can see that for all polycapillary X-ray lenses, the value of l is bigger than zero. In other words, for the synchrotron radiation primary focusing source, the parameter l of the X-ray lens should be bigger than zero.

Table 3. Values of l with different X-ray lenses.

X-ray lens label	1	2	3	4
r_{out}/μm	2.0	2.5	3.0	3.5
The maximum η	39.5%	47.1%	52.5%	55.7%
l/mm	1.1	1.4	1.8	3.0

3.2. Simulated intensity distribution and focal distance

Using the ray-tracing method, we can trace all X-ray transmission in the polycapillary X-ray lens,[6] and we use two-dimensional (2D) and three-dimensional (3D) images to record all X-rays departing from the polycapillary X-ray lens. Figures 5 and 6 illuminate the simulated X-ray 2D images and 3D beam intensity distributions at $f = 15$ mm and 25 mm (f is the distance between the exit of the polycapillary and receiving plane). From the 2D and 3D images, we can see that the X-ray beams are focused in the central zone. The calculated FWHM values with different values of f are shown in Fig. 7. At $f = 15$ mm, the FWHM of the X-ray beam is 183 μm. When the imaging plane is moved away from the polycapillary exit, the FWHM starts to become small. At $f = 25$ mm, the X-ray beam has a minimal focal size. The distance between the exit of the X-ray lens and the minimal focal size position is called the 'focal distance' f_2. So the focal distance for this polycapillary X-ray lens is 25 mm, i.e., $f_2 = 25$ mm. When $f > 25$ mm, the size of the X-ray beam becomes bigger.

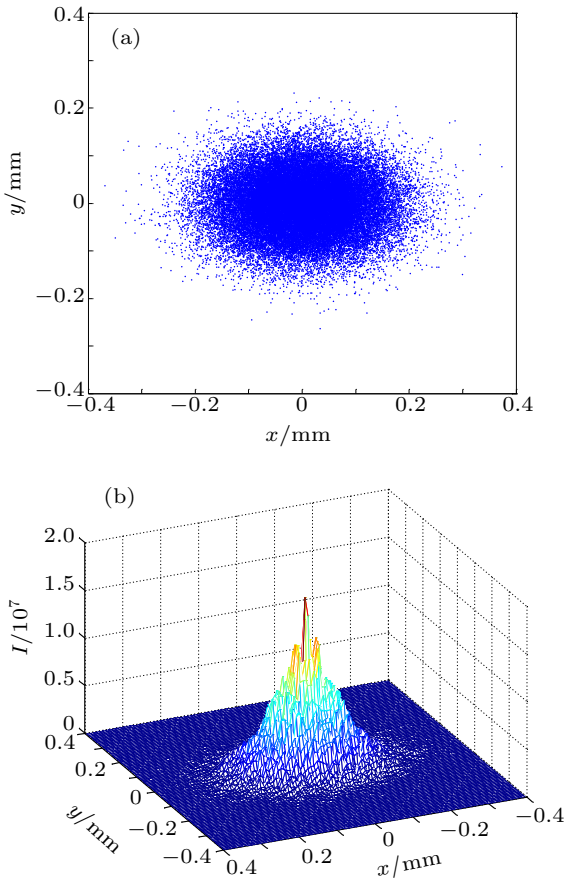


Fig. 5. Simulated X-ray 2D image (a) and 3D beam intensity distribution (b) at the distance $f = 15$ mm.

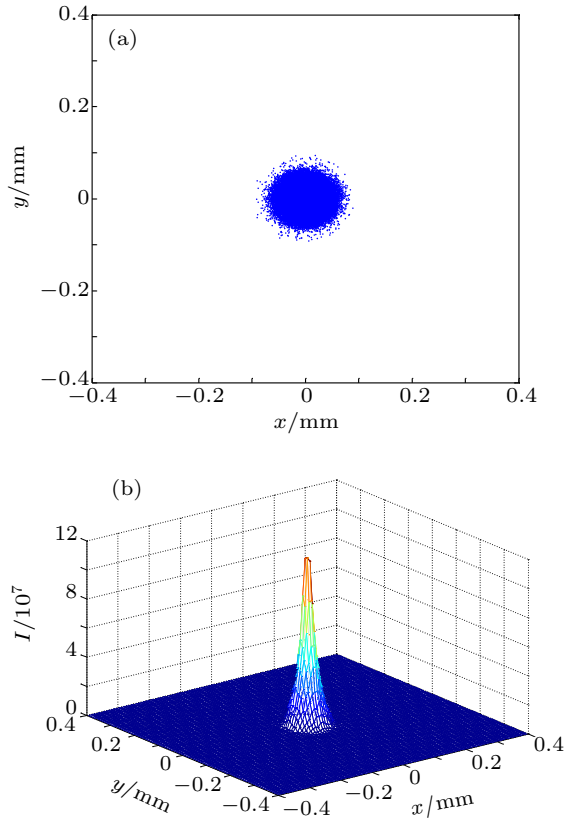


Fig. 6. Simulated X-ray 2D image (a) and 3D beam intensity distribution (b) at the distance $f = 25$ mm.

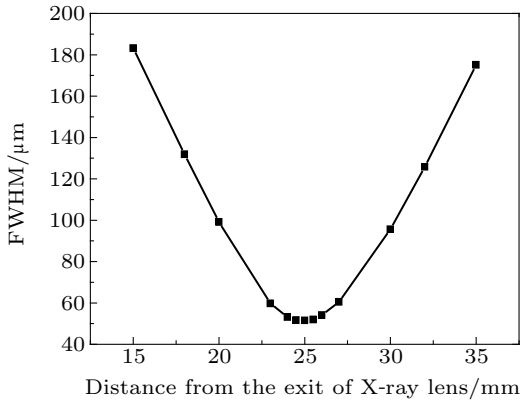


Fig. 7. The FWHMs versus distance from the exit of the X-ray lens.

3.3. Experimental results and discussion

At the Beijing synchrotron radiation biological macromolecule station (1W2B), we measure the transmission efficiencies and the values of f_2 of different polycapillary X-ray lenses. At the same time we acquire the simulation results of the X-ray lens. In order to obtain accurate simulation parameters, we use 3D microscopy (VHX-500) to take photos of the polycapillary X-ray lens end surface. Figure 8 is a photograph of the entrance end of lens No. 11-9-23-2. We can find that the radius of every capillary tube of the entrance end is about 3.8 μm, the radius of the exit end is about 3.0 μm, and the inner radius/outer radius ratio is about 0.78.

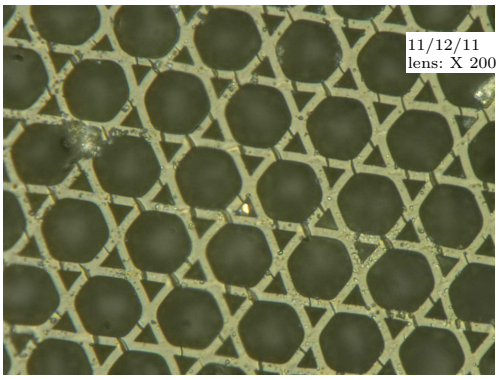


Fig. 8. Entrance photograph of polycapillary X-ray lens (No. 11-9-23-2).

In order to obtain the configuration curve of the polycapillary X-ray lens, we use a high-precision digital micrometer to measure the X-ray lens configuration, and the measuring accuracy is 2 μm. Figure 9 shows the measured configuration curve.

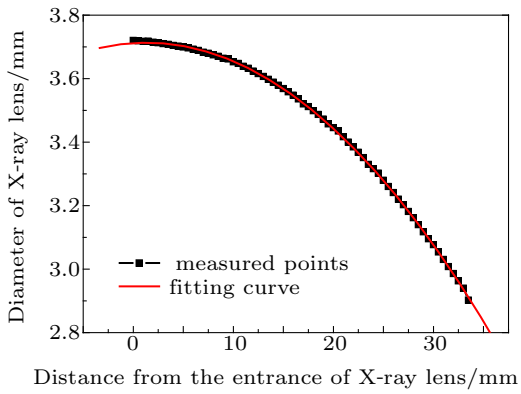


Fig. 9. Configuration curve of polycapillary X-ray lens (No. 11-9-23-2).

Table 4 shows the experimental and theoretical results of X-ray lens transmission efficiency. The simulation parameters are the same as those of the polycapillary X-ray lens. We can see that the theoretical transmission efficiency is larger than the experimental results for the two lenses. The reason for this is that in the simulation model of the polycapillary X-ray lens, the inner surface roughness of each capillary is not taken into account.

Table 4. Experimental and theoretical results of X-ray lens transmission efficiency for lens Nos. 11-9-23-2 and 03-2-18-5.

No.	Length/mm	r_{in}/μm	r_{out}/μm	Rate	Theoretical results	Experimental results
11-9-23-2	33.5	3.72	2.90	0.78	53.1%	47%
03-2-18-5	49.0	4.23	3.14	0.75	50.1%	44%

In Table 5, the focal distance f_2 values of four polycapillary X-ray lenses are listed. The theoretical results are obtained by the same method as that in Subsection 3.2. The experimental results are taken using the metal knife edge scanning method. We can see that the simulation results are very close to the experimental result. The relative error is small.

Table 5. Experimental and theoretical results of the f_2 of different X-ray lenses.

No.	Theoretical results of f_2	Experimental results of f_2	Relative error
03-2-18-5	64	63	2.4%
11-9-6-1	51	53	3.0%
11-9-23-1	27	26	5.9%
11-9-23-2	55	58	5.2%

4. Conclusions

Using the conventional metal knife edge scanning method, we measure the primary focusing spot intensity distribution of the synchrotron radiation source at the Beijing synchrotron radiation biological macromolecule station (1W2B). The measured focusing spot size is 0.86 mm(H)×0.53 mm(V), and the horizontal divergence is 1.6 mrad. According to these data, the theoretical model of the primary focusing source of the Beijing synchrotron radiation biological macromolecule station is established, and this theoretical model is also suitable for the synchrotron radiation source at the other Beijing synchrotron radiation station. At the same time, we use two quadratic functions to establish a mathematical model of the polycapillary X-ray lens. Using the theoretical model of the primary focusing source, we calculate two important parameters – the focal length and transmission efficiency of the polycapillary X-ray lens. We obtain the conclusion that for the primary focusing source of synchrotron radiation, when the l parameter of the X-ray lens is larger than zero, the polycapillary X-ray lens can be chosen to obtain the highest transmission efficiency. We measure the properties of the polycapillary X-ray lens, and the experimental results are in good agreement with the theoretical results.

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