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Optics Communications 280 (2007) 243–248
OPTICS COMMUNICATIONS
www.elsevier.com/locate/optcom

Diffraction transfer function and its calculation of classic diffraction formula

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Received 15 February 2007; received in revised form 8 August 2007; accepted 17 August 2007

Abstract

In scalar diffraction theory, Kirchhoff formula, Rayleigh–Sommerfeld formula, and angular spectrum transmission formula are classic formulas that express diffraction correctly. But as complex calculation, Fresnel diffraction integral, which is the paraxial approximate solution to these formulas, is used widely. This paper presents diffraction transfer function corresponding to each classic diffraction formula, gives discussion on methods when using fast Fourier transform to calculate these formulas, derives conditions each formula must meet when it is calculated correctly based on sampling theorem, and finally real examples are finished to certify the results.

Keywords: Diffraction calculation; Transfer function of diffraction; Fast Fourier transform (FFT)

1. Introduction

In application research on laser, diffraction calculation is a basic research content. According to scalar diffraction theory, Kirchhoff formula, Rayleigh–Sommerfeld formula, and diffraction's angular spectrum transmission formula have already been obtained. Although these formulas are accurate solutions to Helmholtz equation, the complex calculations must be done so that Fresnel diffraction integral, which is the paraxial approximate solution to these formulas, is used actually and widely. Fresnel diffraction integral can be expressed as Fourier transform as well as convolution in mathematical form, and theoretically calculated by Fourier transform and inverse Fourier transform [1]. But usually there are no analytical solutions to these formulas for the practical diffraction, and only can numerical analysis be made using discrete Fourier transform. For long time, diffraction has been one of the most difficult problems in optics [2].

In recent years, with the appearance of fast Fourier transform (FFT) [3] and development of computer techniques, FFT to calculate diffraction on the computer is gradually becoming a popular method. Because the mathematical form of Fresnel diffraction integral is relatively simple, and usually satisfied solutions to practical problems can be obtained, it is still the most widely used formula now. To let the calculations meet Nyquist sampling theorem [3], FFT calculation of Fresnel diffraction integral has been studied widely [4,5].

After all, Fresnel diffraction integral is only the paraxial approximate solution to diffraction problem, there are many restrictions when it is used to resolve some practical problems. It will have vital significance if Kirchhoff formula, Rayleigh–Sommerfeld formula, and diffraction's angular spectrum transmission formula can be calculated fast using FFT. In these three classic formulas, since angular spectrum transmission formula of diffraction has been expressed in terms of transfer function of diffraction concisely, it is easily to be resolved with FFT. However, how to let calculations meet sampling theorem is a question which is worth to be studied. Furthermore, the researches on Kirchhoff formula and Rayleigh–Sommerfeld formula

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doi:10.1016/j.optcom.2007.08.053

have shown that there are transfer functions corresponding to these two formulas, which can also be calculated quickly with FFT [6,7]. Conditions which should be met by each formula when it can be used to calculate diffraction field's amplitude and phase more correctly are derived in this paper based on Nyquist sampling theorem.

Finally the results are certified through diffraction calculation examples.

2. Convolution algorithm of Fresnel diffraction integral

Since the calculation method of classic diffraction formula discussed in this paper is corresponds to the convolution algorithm of Fresnel diffraction integral, in order to be convenient for comparison, initially convolution algorithm is introduced briefly.

Assuming that $U_0\,(x_0, y_0)$ is light wave complex amplitude in the object plane, according to Fresnel diffraction integral, light wave complex amplitude $U\,(x, y)$ arriving at the observation plane with diffractive distance d can be written as [1,2]

$$U(x,y) = \frac{\exp(\mathrm{i}kd)}{\mathrm{i}\lambda d}\int\int_{-\infty}^{\infty} U_0(x_0,y_0)\exp\left\{\frac{\mathrm{i}k}{2d}\left[(x-x_0)^2 + (y-y_0)^2\right]\right\}\mathrm{d}x_0\,\mathrm{d}y_0 \quad (1)$$

where $\mathrm{i} = \sqrt{-1}$ and λ is wavelength with $k = 2\pi/\lambda$.

Assuming that f_x, f_y are coordinates in frequency range, with the help of Fourier transform, the above mentioned equation can be represented as

$$U(x,y) = \mathscr{F}^{-1}\{\mathscr{F}\{U_0(x_0,y_0)\}H_F(f_x,f_y)\} \quad (2)$$

where H_F, called transfer function of Fresnel diffraction [6], can be expressed as

$$H_F(f_x,f_y) = \mathscr{F}\left\{\frac{\exp(\mathrm{i}kd)}{\mathrm{i}\lambda d}\exp\left[\frac{\mathrm{i}k}{2d}(x^2+y^2)\right]\right\} \quad (2a)$$

It is easy to prove that there is an analytical expression of Fresnel diffraction transfer function

$$H_F(f_x,f_y) = \exp\left\{\mathrm{i}kd\left[1-\frac{\lambda^2}{2}(f_x^2+f_y^2)\right]\right\} \quad (2b)$$

Because Eq. (2a) can be calculated directly using FFT, as transfer function, Eqs. (2a) and (2b) are equivalent in theory. Differences between the two equations in practical calculation are given in the latter part of the text.

The calculation form as expressed according to Eq. (2) is usually called diffraction integral's convolution algorithm. The question how to let calculations satisfy sampling theorem is considered now. According to analytical Eqs. (2a) and (2b), because Fresnel diffraction transfer function is a non-band-limited function which has value in the entire frequency domain, it is impossible to make the discrete calculation of Eq. (2) meet Nyquist sampling theorem even if the object function is a band-limited function. However, Nyquist sampling theorem can be described formally that the countdown of spatial range sampling spacing is greater than or equal to double times of function's maximal frequency spectrum. That is to say, there are at least two sampling points in the space period corresponding to the maximal frequency spectrum. In actual diffraction calculation, computations are usually made to meet sampling theorem approximately based on the following analysis [4,5].

When Fresnel diffraction transfer function is expressed as Fourier transform (see Eq. (2a)) in spatial domain, for the given calculation width of diffraction field ΔL_0, there is the largest phase-change rate when x and y are $\Delta L_0/2$ when calculating Fresnel diffraction transfer function by use of FFT. If there are at least two sampling points in the value region when it once changes a 2π period, then FFT calculation is thought to meet sampling theorem approximately. That is

$$\left|\frac{\partial}{\partial x}\frac{\pi}{\lambda d}(x^2+y^2)\right|_{x,y=\Delta L_0/2} \times \Delta x_0 \leqslant \pi$$

From the above inequality, we obtain

$$\Delta x_0 \leqslant \frac{\lambda d}{\Delta L_0} \quad (3)$$

Eq. (3) is the condition, which meets Nyquist sampling theorem, when using transfer function in Fourier transform form.

When using FFT to calculate Eq. (2b), Fresnel diffraction transfer function, its discrete form can be expressed as

$$H_F(m\Delta f_x, n\Delta f_y) = \exp\left\{\mathrm{i}kd\left[1-\frac{\lambda^2}{2}((m\Delta f_x)^2)\right]\right\} \quad (4)$$

where m, $n = -N/2, -N/2+1, \ldots, N/2-1$.

As the transfer function has the largest phase-change rate when m, $n = \pm N/2$, the condition, which meets sampling theorem, is determined by following inequality:

$$\left|\frac{\partial}{\partial m}\frac{2\pi}{\lambda}d\left[1-\frac{\lambda^2}{2}\left((m\Delta f_x)^2+(n\Delta f_y)^2\right)\right]\right|_{m,n=N/2} \leqslant \pi$$

Put $\Delta f_x = \Delta f_y = \frac{1}{\Delta L_0}$ into the above inequality, we can obtain the condition of sampling when using analytical form's Fresnel diffraction transfer function as

$$\Delta x_0 \geqslant \sqrt{\lambda d/N} \quad (5)$$

Comparing Eq. (5) with Eq. (3), it is obvious that Eq. (3) is a more harsh condition. For example, when diffractive distance d is small, the result, which meets sampling theorem, can be obtained only by making the sampling spacing closer to wavelength magnitude. According to the feasibility of numerical calculation, analytical transfer function is better than Fourier transform form's.

Formally, condition (5) seems to have been met very easily. But it must be remembered that this condition is obtained under the precondition that sampling spacing of object function Δx_0 has already satisfied sampling theorem. That is for the given N, λ, and d, Δx_0 cannot be extended arbitrarily.

It must be pointed out that wave light's diffraction is a superposition of angular spectrum's diffraction of wave light field. With the increase of diffractive distance, the range of diffraction field will expand linearly. As in convolution algorithm, the object plane and the observation plane have the same sampling width [4], diffraction field cannot be obtained fully by convolution algorithm when diffractive distance is large. Therefore, this algorithm is mainly used in the situation in which high frequency angular spectrum of object wave light field is small and diffractive distance is small.

3. Diffraction's Kirchhoff transfer function and its calculation

It is easy to prove that Kirchhoff's diffraction formula can be expressed as [6,7]

$$U(x,y) = \mathscr{F}^{-1}\{\mathscr{F}\{U_0(x,y)\}H_J(f_x,f_y)\} \tag{6}$$

where

$$H_J(f_x,f_y) = F\left\{\frac{\exp\left[\mathrm{i}k\sqrt{d^2+x^2+y^2}\right]}{\mathrm{i}2\lambda\left(d^2+x^2+y^2\right)}\left(\sqrt{d^2+x^2+y^2}+d\right)\right\} \tag{6a}$$

is Kirchhoff transfer function of diffraction.

According to the above discussion on Fresnel diffraction integral, the sampling of Kirchhoff transfer function must be considered mainly.

From the analysis of Eq. (6a), spatial change rate of $\exp\lfloor \mathrm{i}k\sqrt{d^2+x^2+y^2}\rfloor$ is much higher than that of $\frac{\sqrt{d^2+x^2+y^2}+d}{\mathrm{i}2\lambda\left(d^2+x^2+y^2\right)}$. As long as the sampling of exp $\lfloor \mathrm{i}k\sqrt{d^2+x^2+y^2}\rfloor$ meets the sampling theorem, the entire transition function's sampling also meets sampling theorem approximately. Therefore, the condition to meet Nyquist sampling theorem can be determined by the following inequality:

$$\left|\frac{\partial}{\partial x}\frac{2\pi}{\lambda}\sqrt{d^2+x^2+y^2}\right|_{x,y=\Delta L/2} \times \Delta x_0 \leqslant \pi \tag{7}$$

which leads to

$$\Delta x_0 \leqslant \frac{\lambda\sqrt{d^2+\Delta L^2/2}}{\Delta L} \tag{8}$$

Therefore, Eq. (8) is the condition for calculation of Kirchhoff formula to meet the sampling theorem.

The above inequality can be simplified as $\Delta x_0 \leqslant \frac{\lambda}{\sqrt{2}}$ when diffractive distance d is very small and $d^2 \ll \Delta L^2/2$ is valid. This conclusion indicates that for small diffractive distance, in order to meet sampling theorem, sampling width must be close to the order of wavelength when using Kirchhoff transfer function to calculate diffraction. It will create great difficulties in actual numerical calculations.

4. Diffraction's Rayleigh–Sommerfeld transfer function and its calculation

Rayleigh–Sommerfeld formula of diffraction can be written as [6,7]

$$U(x,y) = \mathscr{F}^{-1}\{\mathscr{F}\{U_0(x,y)\}H_R(f_x,f_y)\} \tag{9}$$

where

$$H_R(f_x,f_y) = \mathscr{F}\left\{d\,\frac{\exp\left[\mathrm{i}k\sqrt{d^2+x^2+y^2}\right]}{\mathrm{i}\lambda(d^2+x^2+y^2)}\right\} \tag{9a}$$

is Rayleigh–Sommerfeld transfer function.

According to the above discussion on the calculation of Kirchhoff formula, the sampling of function exp $\lfloor \mathrm{i}k\sqrt{d^2+x^2+y^2}\rfloor$ should mainly be considered in the correct discrete calculation. That is, the sampling condition in the calculation of Rayleigh–Sommerfeld formula is the same as that of Kirchhoff formula.

$$\Delta x_0 \leqslant \frac{\lambda\sqrt{d^2+\Delta L^2/2}}{\Delta L} \tag{10}$$

For small diffractive distance, in order to meet the sampling theorem, sampling width must be close to the order of wavelength when using Rayleigh–Sommerfeld transfer function to calculate diffraction, and therefore, the algorithm mentioned above is not usually used in near-field diffraction's calculation.

5. Diffraction's angular spectrum transfer function and its calculation

Based on angular spectrum diffraction theory, the precise solution of diffraction field without the near-axis approximation is expressed in Fourier transform form as

$$U(x,y) = \mathscr{F}^{-1}\{\mathscr{F}\{U_0(x,y)\}H_B(f_x,f_y)\} \tag{11}$$

where

$$H_B(f_x,f_y) = \exp\left[\mathrm{i}kd\sqrt{1-(\lambda f_x)^2-(\lambda f_y)^2}\right] \tag{11a}$$

is angular spectrum transfer function.

Using fast Fourier transform (FFT) and inverse fast Fourier transform (IFFT) to calculate Eq. (11) with sampling width of object plane of ΔL_0 and sampling number of $N\times N$ and sampling spacing $\Delta x_0 = \Delta y_0 = \Delta L_0/N$, Eq. (11) can be represented as

$$U(p\Delta x, q\Delta y) = \mathrm{IFFT}\Big\{\mathrm{FFT}\{U_0(r\Delta x_0 s\Delta y_0)\} \times \exp\left[\mathrm{i}kd\sqrt{1-(\lambda m\Delta f_x)^2-(\lambda n\Delta f_y)^2}\right]\Big\} \tag{12}$$

where p, q, r, s, m, $n = -N/2, -N/2+1, \ldots, N/2-1$.

Using the above discussed method and assuming that discrete transfer function's sampling rate of change is less than or equal to π when m, $n = N/2$, we obtain

$$\left|\frac{\partial}{\partial m}kd\sqrt{1-(\lambda m\Delta f_x)^2-(\lambda n\Delta f_y)^2}\right|_{m,n=N/2}\leqslant \pi.$$

From the above inequality with conditions $\Delta f_x = \Delta f_y = \frac{1}{\Delta L_0}$ and $k = 2\pi/\lambda$, we can obtain

$$\frac{\lambda dN}{\Delta L_0\sqrt{\Delta L_0^2 - 2(\lambda N/2)^2}} \leqslant 1 \tag{13}$$

As $\Delta L_0^2 \gg 2(\lambda N/2)^2$ is usually satisfied, a better approximation of the above inequality is

$$\Delta L_0 \geqslant \sqrt{N\lambda d} \tag{14}$$

The above two inequalities provide the basis for sampling calculation of angular spectrum transmission formula.

Dividing Eq. (14) by N, it becomes $\Delta x_0 \geqslant \sqrt{\lambda d/N}$. Comparing it with Eq. (5), we can see that calculation formula defined by diffraction's angular spectrum transmission theory basically has the same sampling condition as that by using analytical form's Fresnel diffraction transfer function.

6. Calculation examples

To certify the viability of calculation methods mentioned above, we have done an experiment with CO_2 laser of wavelength 10.6 μm. Fig. 1 is the illustration of the experiment. The incident plane is a cross aperture which is made by welding tinsels with diameter 1 mm on a metal plate with a diameter of 60 mm. The incident laser is a standard base mode Gaussian beam with the radius 7.2 mm and power of 500 W. Heat sensitive paper [6] is used to sample the beam at different diffractive distances on the testing screen, and the sampling time is always 15 ms.

According to the experiment, the wave light field which just passes through the cross filament can be expressed as

$$U_0(x_0,y_0) = \mathrm{circ}\left(\frac{\sqrt{x_0^2+y_0^2}}{r}\right)\sqrt{\frac{2P_0}{\pi w^2}}\exp\left(-\frac{x_0^2+y_0^2}{w^2}\right) \times \exp\left(\mathrm{i}k\frac{x_0^2+y_0^2}{2R}\right)\sum_{q=1}^{4}\mathrm{rect}\left(\frac{x_0-x_q}{r},\frac{y_0-y_q}{r}\right) \tag{15}$$

where $r = 30$ mm which is the opening radius of aperture, and

$$x_1 = \frac{r+1}{2},\quad y_1 = \frac{r+1}{2},\quad x_2 = -\frac{r+1}{2},\quad y_2 = \frac{r+1}{2}$$

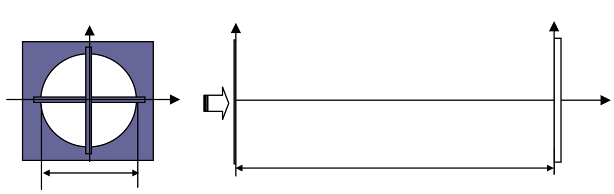

Fig. 1. Laser diffraction experiment on an aperture with a cross filament.

$$x_3 = -\frac{r+1}{2},\quad y_3 = -\frac{r+1}{2},\quad x_4 = \frac{r+1}{2},\quad y_4 = -\frac{r+1}{2}$$

Letting $\Delta L_0 = 20$ mm and $N = 256$, the expression of object plane's wave light field is put into different diffraction calculation formulas. Figs. 2–4 show sampling spots sampled by heat sensitive paper and theoretically stimulating results at the distance of 36 mm, 195 mm and 572 mm, respectively. In these images we can see that results calculated by different transfer functions are significantly different from each other when diffractive distance is relatively small. It is easy to find that the calculated results are deviated greatly from the experimental results when transfer function cannot be expressed as analytical solution in frequency range. According to the analysis on whether each calculation meets sampling theorem, some discussions on the calculated results above are made.

In the case of FFT calculation of Fresnel transfer function, multiplying Eq. (2) by N and considering $N\Delta x_0 = \Delta L$, the condition which meets Nyquist sampling theorem can be written as

$$\Delta L_0 \leqslant \sqrt{N\lambda d} \tag{16}$$

Putting the corresponding parameters in Figs. 2–4 into the above mentioned inequality, we obtain:

$d = 36$ mm : $\sqrt{256\times 0.0106\times 36} = 9.88 < \Delta L_0$,
not meeting sampling theorem;

$d = 95$ mm : $\sqrt{256\times 0.0106\times 95} = 16.05 < \Delta L_0$,
not meeting sampling theorem;

$d = 572$ mm : $\sqrt{256\times 0.0106\times 572} = 39.40 > \Delta L_0$,
meeting sampling theorem.

In the case of Kirchhoff transfer function and Rayleigh–Sommerfeld transfer function, multiplying Eq. (10) by $N\Delta L$ and considering $N\Delta x_0 = \Delta L$, the condition which meets Nyquist sampling theorem can be written as

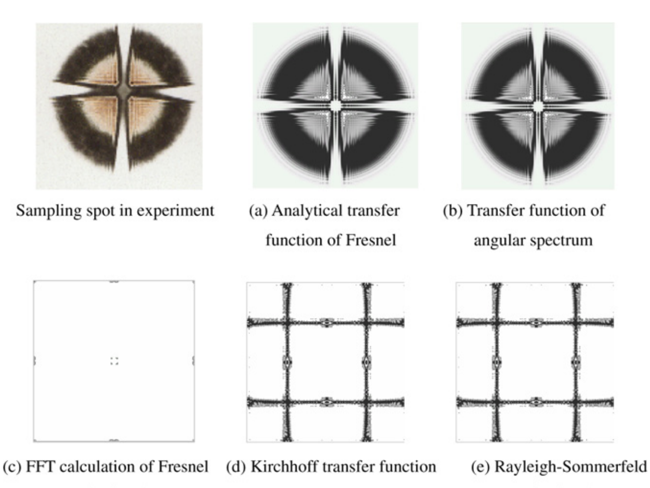

Fig. 2. Comparison of various calculating methods at diffractive distance $d = 36$ mm.

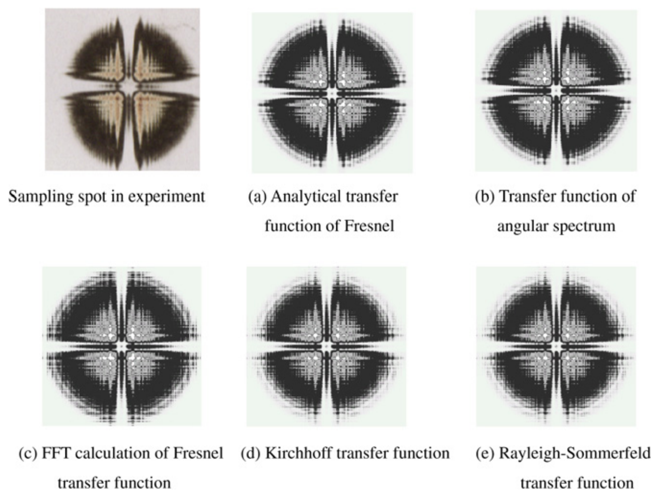

Fig. 3. Comparison of various calculating methods at diffractive distance $d = 95$ mm.

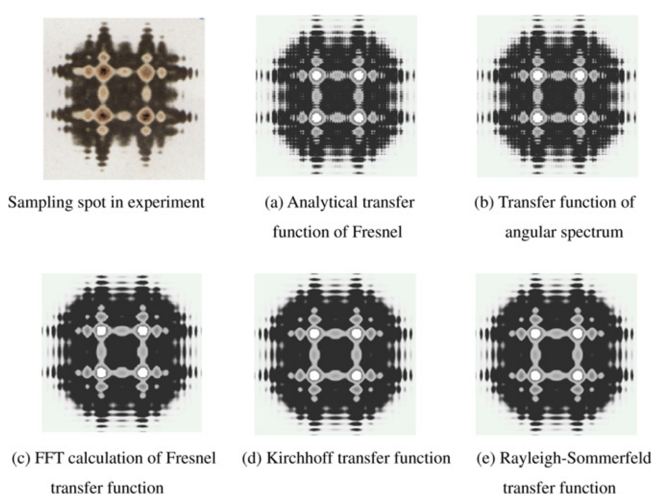

Fig. 4. Comparison of various calculating methods at diffractive distance $d = 572$ mm.

$$\Delta L^2 \leqslant N\lambda\sqrt{d^2 + \Delta L^2/2} \tag{17}$$

Putting the corresponding parameters in Figs. 2–4 into the above mentioned inequality, we obtain:

$$d = 36\ \text{mm} : 256 \times 0.0106\sqrt{36 \times 36 + 20 \times 20/2}$$
$$= 104.7 < \Delta L^2,\ \text{not meeting sampling theorem;}$$
$$d = 95\ \text{mm} : 256 \times 0.0106\sqrt{95 \times 95 + 20 \times 20/2}$$
$$= 260.6 < \Delta L^2,\ \text{not meeting sampling theorem;}$$
$$d = 572\ \text{mm} : 256 \times 0.0106\sqrt{572 \times 572 + 20 \times 20/2}$$
$$= 1552.65 > \Delta L^2,\ \text{meeting sampling theorem.}$$

Above calculations indicate that for FFT calculation of Fresnel transfer function, Kirchhoff transfer function and Rayleigh–Sommerfeld transfer function, only the calculations with $d = 572$ mm meet Nyquist sampling theorem approximately.

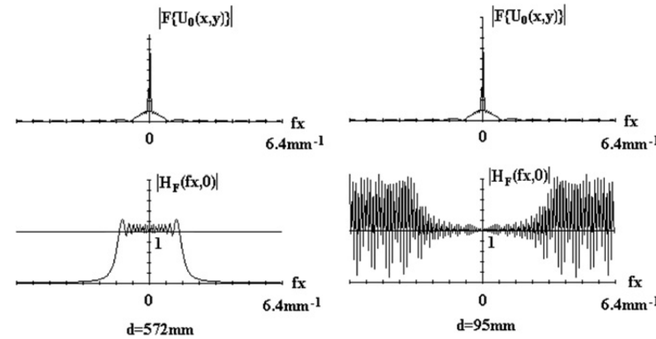

Fig. 5. Frequency spectrum of object wave and amplitude–frequency response curves of Fresnel transfer function calculated through FFT at $d = 572$ mm and $d = 95$ mm.

Formally, the calculation with $d = 95$ mm (as shown in Fig. 3) seems to lead to correct results, but this is because of the coincidence that frequency spectrum section of FFT calculation of transfer function, when it is used to reflect characteristics of object function, is accidentally close to the correct values. For the sake of visualization, Fig. 5 shows a frequency response curve of object function and frequency response curves obtained by FFT calculation of Fresnel transfer function with $d = 572$ mm and $d = 95$ mm respectively.

According to the analysis of these two curves, it is not difficult to see that the transfer function for the diffractive distance of 572 mm is a low-pass filter with a module approximately close to 1 in low frequency region (Fig. 5 shows an angular spectrum transfer function curve with the module of 1 as a reference). Frequency spectrum of diffraction field is obtained by multiplying the main part of object light frequency spectrum with transfer function. Then diffraction field with a part of high spatial frequency losses can be obtained by using discrete inverse Fourier transform. But when $d = 95$ mm, there will be a strong frequency spectrum superposition in FFT calculation of transfer function due to insufficient sampling, and there will be a complex distribution with the module lager than 1in high frequency region, which will lead to energy amplification of object function's transition in high frequency spectrum region and result in distortion eventually. However, object function's frequency spectrum corresponding to frequency spectrum's superposition region is just close to zero, and the product of the frequency spectrum of object light and the transfer function remains very small, which does not have a significant influence on the frequency spectrum of diffraction field. Therefore, although FFT calculation of transfer function for $d = 95$ mm does not meet Nyquist sampling theorem, diffraction calculation results which are close to practical situation can be also obtained. In actual calculation, the opportunity mentioned above is very small. In order to obtain reliable calculations, the reliability of calculations must be judged according to the related discussion on Nyquist sampling theorem.

7. Discussion and results

According to scalar diffraction theory [1,2], all of diffraction's angular spectrum transmission formula, Kirchhoff formula and Rayleigh–Sommerfeld formula are equivalent expressions of the same physical problem in spatial range and frequency range. The difference between them is that the transfer function of Kirchhoff and Rayleigh–Sommerfeld can be expressed only by Fourier transform. When diffractive distance is relatively small and sampling is insufficient, there will be big errors in Kirchhoff transfer function and Rayleigh–Sommerfeld transfer function, when using FFT to calculate practical diffraction problems. The reason is not that Kirchhoff transfer function and Rayleigh–Sommerfeld transfer function themselves is wrong, but the question of insufficient sampling has made natures of discrete function change a lot from its original function when using FFT sampling to calculate transfer function. If discrete function cannot represent the original function, the results will surely not be correct. There is no conclusion about Kirchhoff formula and Rayleigh–Sommerfeld formula, as to which one is more accurate [1,2]. Transfer functions and discussion on how to make transfer function meet sampling theorem given in this paper provide a possible way to the further study on these two formulas.

Moreover, from the sampling study on transfer functions of different forms above, it can be seen that diffraction's angular spectrum transmission function usually is more effective than the other transfer functions for the same calculating problem. And from sampling number and calculation time, it is easy to confirm that their calculations are basically the same as that of analytical transfer function of Fresnel diffraction, and accurate solutions to diffraction problems can be obtained in theory. Therefore, using angular spectrum diffraction formulas as far as possible should be able to obtain more reliable results in practical applications.

This work was supported by Nation Natural Science Foundation of China (60178004) and the Natural Science Foundation of Yunnan Province (2004F0025M).

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