



Numerical visualization of aperiodic scalar optical wave fields

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Abstract: In numerical wave optic simulations using the conventional angular spectrum method, numerical inter-periodic interference occurs as a result of the inherent periodicity of the discrete Fourier transform. In this paper, we propose an aperiodic angular spectrum representation of a scalar optical wave field without numerical inter-periodic interference in an aperiodic area. The visualization of holographic three-dimensional image light field is presented for the validity of the proposed method. It is believed that the proposed method can be broadly applied to visualization of scalar optical wave field represented by the angular spectrum plane wave bases.

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OCIS codes: (050.1755) Computational electromagnetic methods; (070.0070) Fourier optics and signal processing; (050.1960) Diffraction theory.

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1. Introduction

The numerical simulation of scalar optical waves is a fundamental problem in optical engineering [1]. The numerical model of scalar wave field in free space is crucial as the main theoretical tool for various optical engineering topics such as holographic three-dimensional (3D) display [2, 3], holographic microscopy [4–7], wave-optic based dispersive spectrometer [8], and free space communication [9]. Although the fundamental analytic theory for scalar optical field in free space was already established, regarding numerical modeling 3D visualization of scalar optical wave fields, we have much room to research in numerical domain further because of practical limit in computational resource.

In this paper, we address a theoretical issues associated to the numerical modeling of scalar wave field in free space. The angular spectrum representation is the most popular formula for optical wave propagation in free space and known as a perfect analytic solution of arbitrary free space optical scalar wave field. In practice, the numerical model derived from the angular spectrum representation is calculated and visualized in the discrete spatial sampling grids [10, 11]. Theoretically, the angular spectrum representation is the linear and coherent superposition of infinitely extended plane wave basis with complex amplitude. In continuum, the analytic angular spectrum representation is a perfect solution of scalar wave equation in free space, however, when the spatial domain is discretized and finite-sized, the basic assumption of using infinitely extended plane wave basis and its validity becomes questionable. In practice, the inter-periodic interference that appears in the direct numerical simulation of the conventional angular spectrum representation of aperiodic scalar optical wave fields is problematic. In this paper, its cause is analyzed and a candidate solution for this issue is proposed. The proposed method is based on the famous Sommerfeld analysis of half-infinite diffraction [12]. An alternative form of the angular spectrum representation using the sommerfeld half-infinite diffraction wave function as the wave function basis is developed, which seems to be quite different from the conventional angular spectrum representation using infinite plane wave basis. For the validation of the proposed formula, we present a comparative study of numerical reconstructions of complex digital hologram using the proposed method and the conventional methods.

The paper is organized as follows. In section 2, the inter-periodic interference in conventional angular spectrum representation is addressed and its cause is analyzed. In section 3, a numerical method for numerical visualization of aperiodic scalar optical wave field is proposed and the numerical simulation results of digital hologram reconstruction are presented. The concluding remarks are followed in section 5.

2. Inter-periodic interference in conventional angular spectrum representation

The scalar wave equation in free space is

$$\nabla^2 U(x, y, z) + k_0^2 U(x, y, z) = 0, \quad (1)$$

where k_0 is the wavenumber $k_0 = 2\pi / \lambda$. Numerical modeling methods for this theory have been the subject of a great deal of research. In Fourier optics [1] and scalar optical wave propagation has been theoretically established. Various mathematical formulations of $U(x, y, z)$ such as the Rayleigh-Sommerfeld formulation and the angular spectrum representation, are well-known. In particular, the angular spectrum representation is a rigorous and versatile formula for the numerical calculation of $U(x, y, z)$ and various applications based on scalar wave optic theory. The optical field $U(x, y, z)$ is represented by the following analytic formula in 3D space,

$$U(x, y, z) = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A(k_x, k_y) e^{j\sqrt{(k_0)^2 - k_x^2 - k_y^2}z} e^{j(k_x x + k_y y)} dk_x dk_y, \quad (2)$$

where $A(k_x, k_y)$ is the angular spectrum of $U(x, y)$. The form of the total field is interpreted to be the coherent superposition of many plane waves with their own direction in 3D space and complex amplitude $A(k_x, k_y)$. The total field $U(x, y, z)$ can be decomposed into propagating and evanescent components, which are partial integrals in the range of $k_x^2 + k_y^2 \leq k_0^2$ and $k_x^2 + k_y^2 > k_0^2$ given, respectively, by

$$U_{pro}(x, y, z) = \frac{1}{4\pi^2} \iint_{k_x^2 + k_y^2 \leq k_0^2} A(k_x, k_y) e^{j\sqrt{(k_0)^2 - k_x^2 - k_y^2}z} e^{j(k_x x + k_y y)} dk_x dk_y, \quad (3)$$

$$U_{eva}(x, y, z) = \frac{1}{4\pi^2} \iint_{k_x^2 + k_y^2 > k_0^2} A(k_x, k_y) e^{-\sqrt{(k_0)^2 - k_x^2 - k_y^2}z} e^{j(k_x x + k_y y)} dk_x dk_y. \quad (4)$$

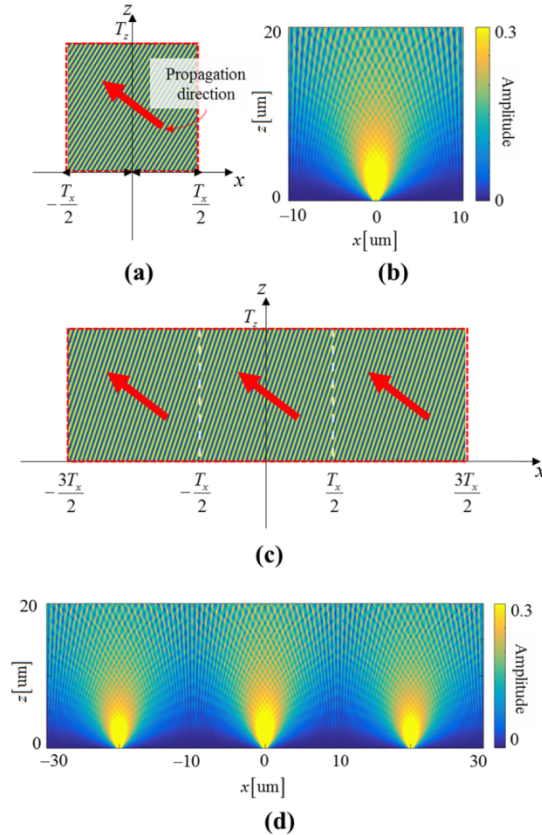


Fig. 1. Optical field visualization using the conventional angular spectrum method: (a) a uniform directional plane wave basis in a rectangular computation region, (b) diffraction field $U(x, y, z)$ for a single slit aperture contaminated by numerical inter-periodic interference, (c) a plane wave basis and (d) diffraction field distribution extended in three-period domain. In (b) and (d), each slit has a width of $5 \mu\text{m}$, and the wavelength is set to 633 nm . In (c) and (d), the x-axis period for the unit computational domain is set to $20 \mu\text{m}$.

The propagating component $U_{pro}(x, y, z)$ is distributed within the free space region, while the evanescent component $U_{eva}(x, y, z)$ is tightly bound near $z = 0$ and does not extend to the free space. In numerical computation, the angular spectrum representation is modeled by $U(k\Delta x, l\Delta y, q\Delta z)$,

$$U_{pro}(p\Delta x, l\Delta y, q\Delta z) = \frac{\Delta k_x \Delta k_y}{4\pi^2} \sum_{n=-\frac{N-1}{2}}^{\frac{N-1}{2}} \sum_{m=-\frac{M-1}{2}}^{\frac{M-1}{2}} A(m\Delta k_x, n\Delta k_y) e^{j\sqrt{(k_0)^2 - (m\Delta k_x)^2 - (n\Delta k_y)^2} q\Delta z} e^{j(m\Delta k_x p\Delta x + n\Delta k_y l\Delta y)}, \quad (5)$$

where Δx and Δy are the sampling intervals in the x-y spatial domain. Δk_x and Δk_y are those in the x-y spatial frequency domain, M and N indicate the number of samples in the x-y spatial frequency domain, which is usually set to an odd number to preserve the origin point of this domain. In practice, Eq. (5) can be efficiently calculated using the fast Fourier transform (FFT). For this, Δk_x and Δk_y are taken by $\Delta k_x = 2\pi / T_x$ and $\Delta k_y = 2\pi / T_y$, where T_x and T_y are the x- and y-direction widths of the computation region, respectively. The discrete angular spectrum Eq. (5) leads to a periodic pattern in the spatial domain due to the periodicity of the Fourier series. This periodicity produces numerical inter-periodic interference patterns in the resulting field visualization. For example, let us consider the optical field for a single slit aperture under normal incidence, $U(x)$, which is given by

$$U(x) = U_0 \text{rect}(x/W). \quad (6)$$

Figure 1 presents the numerical simulation result for the aperture diffraction using the angular spectrum representation of Eq. (5). The uniform plane wave basis in the computation region and the diffraction field contaminated by inter-periodic interference are shown, in Figs. 1(a) and 1(b), respectively. The plane wave basis completely fills the rectangular computation region and this is assumed to induce the periodicity shown in Fig. 1(c). This means that the coherent superposition of the infinitely extended plane wave bases in Eq. (5) produces the total optical field distribution shown in Fig. 1(d). Infinitely extended plane wave bases influence the entire computational space, preventing the numerical isolation of computational sections. This strong interference pattern is a problem when we want to simulate real single slit diffraction.

3. Aperiodic angular spectrum representation without inter-periodic interference

In order to address the inter-periodic interference issue, many numerical electromagnetic simulation techniques such as the finite different time domain (FDTD) method and the Fourier modal method (FMM) employ a perfectly matched layer (PML). The PML is a necessary tool for numerical isolation in aperiodic structure analysis [13,14]. To our knowledge, an effective PML for the scalar wave equation has yet to be proposed. This means that a scalar angular spectrum method for aperiodic wave field representation has not yet been developed for Fourier optics. The half-infinite barrier can play the same role of the PML for aperiodic visualization of scalar optical wave fields. To present aperiodic plane wave basis instead of the infinite plane wave basis, we employ the approach of the modified theory of physical optics (MTPO) [15,16]. The MTPO wave function is the modified representation of the Sommerfeld half-infinite diffraction field. The function of the barrier can be understood in terms of a zero-thickness analytic PML effectively rejecting in-coming wave fields through the vertical side-wall. For a vertical half-infinite barrier ($0 \leq z \leq \infty$, $x = -T_x/2$), one of the angular spectrum wave bases for the longitudinal angle θ_0 , which corresponds to

$e^{jk_x x} e^{j\sqrt{(k_0)^2 - k_x^2} z}$, is generated in the manner illustrated in Fig. 2(a). The rotation of the volumetric field of the reference basis with the azimuthal angle ϕ_0 generates the necessary complete angular spectrum basis in 3D space corresponding to $e^{j(k_x x + k_y y)} e^{j\sqrt{(k_0)^2 - k_x^2 - k_y^2} z}$, as shown in Fig. 2(b). The rotational trajectory of the half-infinite barrier, therefore, specifies the computation volume in the cylindrical volume space as shown in Fig. 2(c).

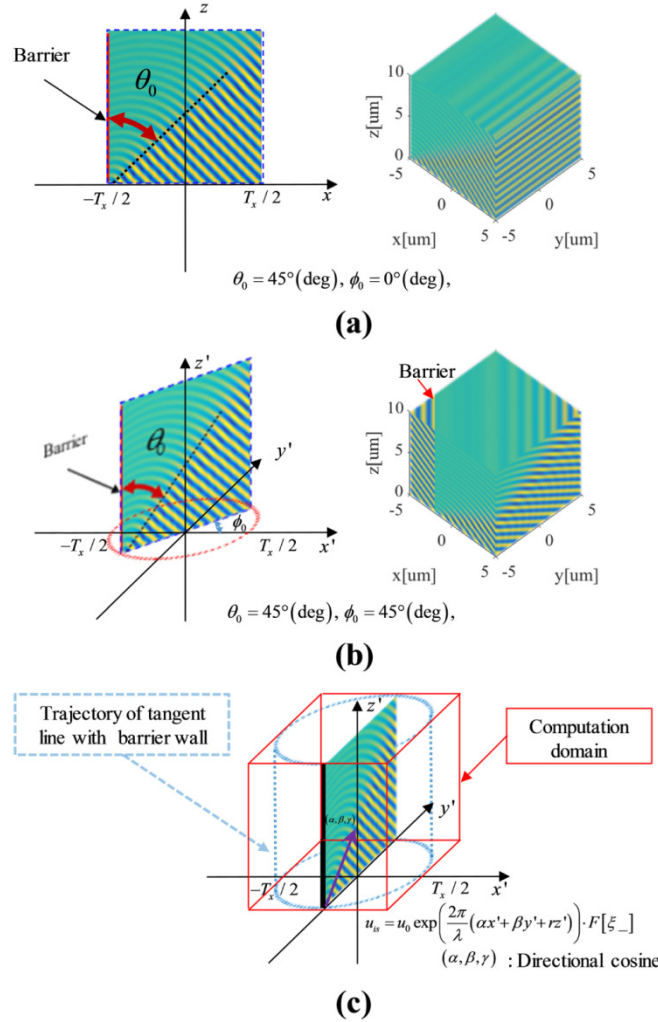


Fig. 2. Numerical structure of the proposed aperiodic angular spectrum representation using an MTPO wave function for a half-infinite plane: (a) diffraction wave departing from a finite bottom region with a vertical half-infinite barrier ($0 \leq z \leq \infty$, $x = -T_x/2$), (b) diffraction wave rotated by the azimuthal angle ϕ_0 , and (c) the cylindrical computation volume for the aperiodic angular spectrum representation.

With this wave basis generation algorithm, we can complete the set construction of the 3D angular spectrum wave basis and can span the general arbitrary scalar wave field in an isolated cylindrical volume of free space. An alternative to the wave basis is the Sommerfeld solution for the black half-plane problem with a perfect absorber [12]. Interestingly, the Sommerfeld solution with a black half plane is an exact equivalent to the incident scattered

field in the MTPO solution for a perfect conducting half plane [15–17]. The only difference is the weighting of the phase $\sqrt{\sin \theta'_0}$. For $\theta'_0 = \pi/2$, these formulas are the same. From Ref [16], the analytic formula for the incident scattered field of an MTPO wave function with a half-infinite barrier ($0 \leq z \leq \infty$, $x = -T_x/2$) for $\mathbf{k} = (k_0 \sin \theta_0, 0, k_0 \cos \theta_0)$ is given as

$$u_{is}(P) = u_0 \exp[jk_0\{(x+T_x/2)\sin\theta_0 + z\cos\theta_0\}] \cdot F[\xi_-], \quad (7)$$

where, P is the observation point (x, y, z) , and the function $F[\cdot]$ denotes the Fresnel integral represented by

$$F[\chi] = \frac{e^{j/\pi^4}}{\sqrt{\pi}} \int_{\chi}^{\infty} e^{-j\tau^2} d\tau, \quad (8)$$

and ξ_- is expressed by

$$\xi_- = -\sqrt{k_0} \sqrt{\left(z^2 + (x+T_x/2)^2\right)^{1/2} + z\cos\theta_0 + (x+T_x/2)\sin\theta_0} \times S\left[\tan^{-1} \frac{-(x+T_x/2)}{z}, \theta_0\right]. \quad (9)$$

In Eq. (9), $S[\cdot]$ is the internal sign function and can be represented by

$$S[\theta, \theta_0] = -\text{sign}(\theta - (\pi - \theta_0)) \cdot \text{sign}((3\pi - \theta_0) - \theta) \quad (10)$$

The basis for the angular spectrum is generated by rotating the reference wave function Eq. (7) by the azimuthal angle ϕ_0 . Therefore, the proposed angular spectrum method uses a rotated MTPO wave function basis in contrast to the conventional angular spectrum method, which uses an infinite plane wave basis. By taking the rotational variable change,

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos\phi_0 & \sin\phi_0 & 0 \\ -\sin\phi_0 & \cos\phi_0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}, \quad (11)$$

we can obtain the rotated MTPO wave function $u_{is}(P)$ for (θ_0, ϕ_0) by

$$u_{is}(P) = u_0 \exp[jk_0\{x'\sin\theta_0\cos\phi_0 + y'\sin\theta_0\sin\phi_0 + z'\cos\theta_0 + (T_x/2) \cdot \sin\phi_0\}] \cdot F[\xi_-] \quad (12)$$

and ξ_- is written as

$$\begin{aligned} \xi_- = & -\sqrt{k_0} \sqrt{\left(z'^2 + (x'\cos\phi_0 + y'\sin\phi_0 + T_x/2)^2\right)^{1/2} + z'\cos\theta_0 + (x'\cos\phi_0 + y'\sin\phi_0 + T_x/2)\sin\theta_0} \\ & \times S\left[\tan^{-1} \frac{-((x'\cos\phi_0 + y'\sin\phi_0 + T_x/2))}{z'}, \theta_0\right]. \end{aligned} \quad (13)$$

Here, one important step remains. The MTPO wave function Eq. (12) has a non-zero phase when compared with the corresponding uniform plane wave $e^{j(k_x x + k_y y + k_z z)}$ at the origin point $P(0, 0, 0)$. The phase compensation term should be multiplied by Eq. (12) so that $u_{is}(\mathbf{0}) = 1$

. The rotated MTPO wave function in Eq. (12) is a complex function consisting of amplitude function $g(P)$ and phase function $h(P)$,

$$u_s(P) = g(P) \cdot \exp(jh(P)). \quad (14)$$

The phase at the origin point can be extracted using the delta function $\beta = h(\mathbf{0}) = \int h(P) \cdot \delta(P) dP$. We can offset the non-zero phase at the origin point as follows,

$$\tilde{u}_s(P) = e^{-j\beta} \times u_s(P). \quad (15)$$

In addition, for the spectrum basis for $\theta_0 = 0(\text{deg})$ or $\mathbf{k} = (0, 0, k_0)$, we take a normal uniform plane wave as the spectrum basis because there is no adapted solution for the MTPO wave function. Consequently, we can complete the construction of the aperiodic angular spectrum basis by solving for k_x and k_y as

$$u_b(x, y, z, k_x, k_y) = \begin{cases} \tilde{u}_s(x, y, z, k_x, k_y), & \text{otherwise} \\ \exp(jk_z z), & k_x = k_y = 0 \end{cases} \quad (16)$$

The MTPO wave function is

$$u_s(x, y, z, k_x, k_y) = u_0 \exp \left[j \left\{ k_x x + k_y y + k_z z + (T_x/2) \cdot \frac{k_y}{\sqrt{k_x + k_y}} \right\} \right] \cdot F[\xi_-] \quad (17)$$

and ξ_- can be expressed by

$$\begin{aligned} \xi_- = & -\sqrt{k_0} \sqrt{\left((z)^2 + \left((k_x x + k_y y) / \sqrt{k_x + k_y} + T_x/2 \right)^2 \right)^{1/2} + z(k_z/k_0) + \left((k_x x + k_y y) / k_0 + T_x \sqrt{k_x + k_y} / (2k_0) \right)} \\ & \times \mathbb{S} \left[z, \left((k_x x + k_y y) / \sqrt{k_x + k_y} + T_x/2 \right), \tan^{-1} \left(\sqrt{k_x + k_y} / k_z \right) \right] \end{aligned} \quad (18)$$

Finally, the aperiodic angular spectrum integral of the 3D wave field takes the form

$$U(x, y, z) = \frac{1}{4\pi^2} \iint_{k_x^2 + k_y^2 \leq k_0^2} A(k_x, k_y) u_b(x, y, z, k_x, k_y) dk_x dk_y + \frac{1}{4\pi^2} \iint_{k_x^2 + k_y^2 > k_0^2} A(k_x, k_y) e^{-\sqrt{k_x^2 + k_y^2 - k_0^2} z} e^{j(k_x x + k_y y)} dk_x dk_y. \quad (19)$$

In Fig. 3, the diffraction field calculated with the proposed aperiodic angular spectrum method in Eq. (19) is compared with that obtained by the conventional angular spectrum method in Eq. (2). It can be seen that, apart from the bottom aperture, the diffraction field in Fig. 3(b) does not reveal the inter-periodic interference pattern, which is contrasted to the appearance of the strong interference patterns in Fig. 3(b). In the simulation, T_x and T_y are set at $10\mu\text{m}$ and a rectangular aperture of $1\mu\text{m}$ by $1\mu\text{m}$ is placed at the origin. The 3D cross-sectional field visualizations of the conventional angular spectrum method and the proposed aperiodic angular spectrum method are shown in Figs. 3(a) and 3(b). The transversal cross-sections of the 3D field distributions for the two methods are compared in Figs. 3(c) and 3(d). As clearly proven in this comparison, the proposed aperiodic angular spectrum method successfully produces an aperiodic 3D scalar wave field without inter-periodic interference. Also, it is worth noting that, in the proposed aperiodic angular spectrum method, the angular

spectrum basis is a solution to the scalar wave equation; therefore, the proposed aperiodic angular representation is also an exact solution to the scalar wave equation. For the evanescent field, the MTPO wave function is not defined. From a physical point of view, the evanescent field is confined to just around the aperture, thus evanescent fields in adjacent computational grids do not considerably interfere with each other, even though the infinitely extended plane wave basis in the evanescent spectrum is used in the numerical modeling. Therefore, the MTPO scattered wave function was only applied to the propagating wave component in the present study.

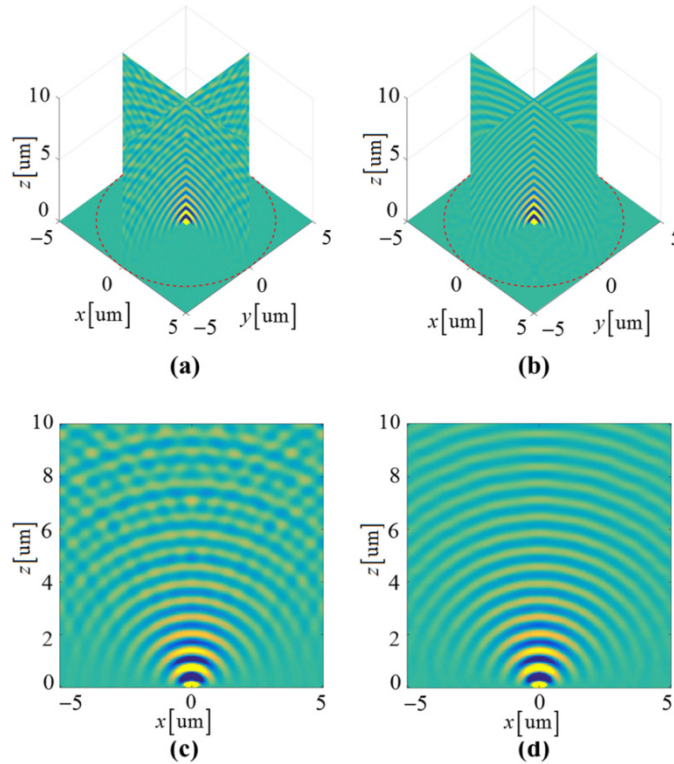


Fig. 3. Cross-sectional plots of $U(x, y, z)$ 3D field visualization of optical wave fields obtained through (a) the conventional angular spectrum method and (b) the proposed aperiodic angular spectrum method. The x - z cross-section field distributions of each method are plotted in (c) and (d) respectively. The dashed red circle at the bottom indicates the trajectory of the tangent point of the barrier wall.

4. Numerical visualization of aperiodic holographic optical fields

In this section, the visualization of holographic optical field is presented for the validity and usefulness of the proposed method. In the fields of digital holography and holographic microscopy, the computational synthesis and reconstruction of digital holograms are the essential wave optic topic. The aforementioned inter-periodic interference causes considerable numerical problems in both of synthesis and reconstruction of digital holograms. Normally, to avoid this problem, computation domain is enlarged so that the inter-periodic interference dose not invade the region of interest. It could be a temporary expedient, but cannot be a sound solution in many practical numerical wave optic simulations.

In Figs. 4(a) and 4(b), the visualizations of scalar diffraction field generated from a periodic binary amplitude grating on a $11\mu\text{m}$ width finite aperture is compared by the conventional angular spectrum method and the proposed aperiodic angular spectrum method.

The period and fill factor of the binary amplitude grating are $1\mu\text{m}$ and 50%, respectively, and a plane wave is incident on the backside of the grating. In the field visualization, the Talbot effect is observed in the mid-field zone where three diffraction orders are spatially overlapped. In Fig. 4(a), the inter-periodic interference contaminates the field distribution and the non-physical Talbot effect appear repeatedly in the area distant from the grating, while the effect of prevention of inter-periodic interference in the proposed method is clearly demonstrated in Fig. 4(b). In Fig. 5, the proposed method is compared to the conventional method in the 3D numerical reconstruction of digital holograms under a holographic microscope setup. A complex hologram pattern is laid on the x - y plane ($z = 0\mu\text{m}$), which displays two axially separated objects in the free space. The first one is a character 'A' positioned at $z = 15\mu\text{m}$ and the second one, character 'B', is positioned at $z = 30\mu\text{m}$. In the simulation, the number of sampling for each x - y plane is 401 by 401, the sampling intervals in x - y plane are $\Delta x, \Delta y = 0.1\mu\text{m}$ and wavelength is $\lambda = 633\text{nm}$. The light energy of the complex hologram pattern in this example is relatively focused around the center of the x - y plane, and the optical field tends to propagate along the z -axis with diverging feature. At $z = 15\mu\text{m}$, the character 'A' is clearly focused, but the character 'B' is out of focus. The optical field distributions that are visualized using the conventional and proposed methods are shown, respectively, in Figs. 4(a) and 4(b), respectively. The optical field distributions at $z = 15\mu\text{m}$ are similar for both cases, however, at $z = 30\mu\text{m}$, the difference between the field visualizations are clearly observed. As seen in Fig. 4(a), the inter-periodic interference occurs at the optical field visualization at $z = 30\mu\text{m}$ in the case of the conventional method. the character 'B' is focused for both cases, but the left part of the diffracted field of the character 'A' invades across the opposite right boundary of the computation domain in the case of the conventional angular spectrum method. While, in the case of the proposed aperiodic angular spectrum method, the perfect aperiodic field visualization without the inter-periodic interference is obtained as shown in Fig. 4(b). In this result, it needs to note that the computation region of the aperiodic angular spectrum is specified by the cylindrical volume whose circumference is determined by the circular trajectory of the half-infinite barrier as mentioned in Fig. 2.

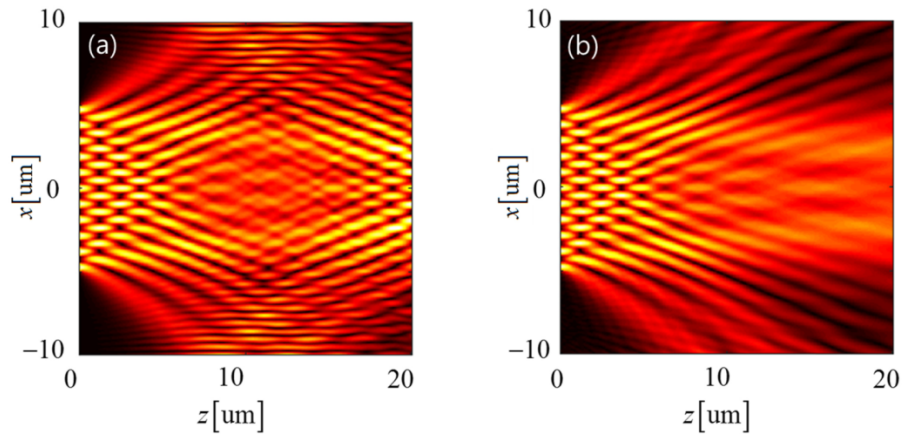


Fig. 4. Numerical reconstruction of diffraction fields from a binary amplitude grating pattern using (a) the conventional angular spectrum method and (b) the proposed aperiodic angular spectrum method. The period and fill factor of the grating pattern are $1\mu\text{m}$ and 0.5, respectively.

The accuracy of the field representation varies with the spatial position of the barrier. As the barrier diameter R increases, the superposition of the wave bases used in the field representation becomes denser and the accuracy in the field calculation associated with the

density of the wave bases at a specific position is improved. As the measurement point is farther from the x - y plane ($z = 0 \mu\text{m}$), the superposition density becomes thinner, meaning that the accuracy of the field representation is degraded. Therefore, the field calculation accuracy is determined by the superposition density of the wave bases and the superposition density is controlled by the radius R of the computational domain $x^2 + y^2 \leq R^2$ and varied with the z -directional position. As for the calculation time, the several steps of assignment, rotation, and multiplication of matrices necessary for the calculation of the MTPO wave function u_{ts} can affect the calculation time of the proposed method. When the number of sampling points are same, the calculation time is estimated to be about three times longer than that of the conventional method. Moreover, the further investigation for the fast calculation algorithm of the MTPO wave function is a necessity.

However, assuming a specific computation grid volume is set up, we can save the MTPO wave function u_{ts} as the basis set by the form of matrices in advance, then the computation load is posed on the linear combination of the pre-calculated bases with specified complex angular spectrum coefficients and the computation efficiency can be enhanced in practice.

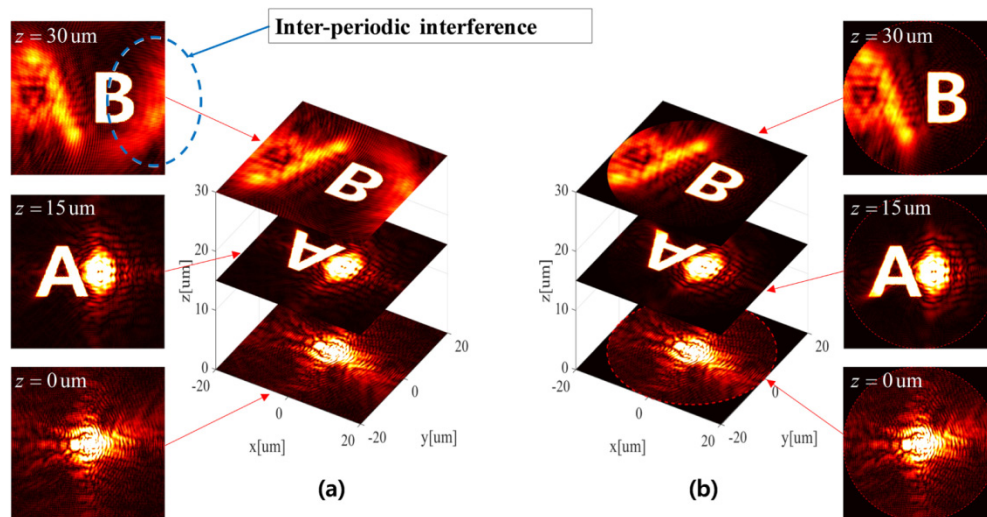


Fig. 5. Numerical reconstruction of a digital hologram using (a) the conventional angular spectrum method and (b) the proposed aperiodic angular spectrum method. The complex hologram pattern is placed at $z = 0 \mu\text{m}$. The target images 'A' and 'B' are focused, respectively, at $z = 15 \mu\text{m}$ and at $z = 30 \mu\text{m}$.

5. Conclusion

In conclusion, we have proposed the aperiodic angular spectrum representation incorporating an analytic thin PML, which might be the first use of a PML for scalar optical waves in Fourier optics. In principle, the proposed method can be widely applied to general optical field models using plane wave bases and Fourier analysis. It is hoped that this method can be extended the method to solve the general inhomogeneous scalar wave equation and visualize aperiodic scalar optical wave field in inhomogeneous media.

Funding Information

This work was supported by Samsung Display Co. Ltd.