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Mathematical methods for holographic mask with layered structure synthesis

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Abstract. In this paper various layered holographic mask structures are proposed and their effectiveness is assessed. A method for diffraction modelling, suitable for use in layered structures of such masks, is proposed. A software module that allows to calculate the transmission and reflection of a plane wave of arbitrary polarization on periodic inhomogeneous medium with a cylindrical structure is developed. This software module is intended to be used for the study of applicability limits of some approximate methods for solving diffraction problems. The developed methods and programs have also been used to solve problems in other fields of electrodynamics, for example, in the problem of ocean surface radiolocation. Mathematical modelling of effects such as Brewster angle and Wood's anomaly was performed with the resulting software module. Quantitative modelling results coincide with the analytical formulas with good accuracy.

1. Introduction

In traditional methods of photolithography, a stencil mask is used, which basically repeats topology of the processor layer in an enlarged form. The size of such mask is about 4-5 times larger than the size of the desired image. In the alternative subwavelength holographic lithography [1-2], which is actively developing at the present time, a binarized holographic mask is used, which is a realization of the transmission function obtained on the basis of the classical principle proposed by D. Gabor [3]. The main property of the hologram is that each element contains some information about all the elements of the object. This, for example, when the information capacity of the hologram is much larger than the amount of information contained in the object, leads to the fact that almost complete information about the object can be restored with the help of a small part of the hologram or with the aid of a damaged hologram. This property of the hologram advantageously distinguishes the holographic mask from the stencil mask, any local defect on which will be reproduced in the image.

The simplest version of the holographic mask structure is an opaque chrome screen on a quartz substrate with rectangular holes of variable size, centres of which are arranged along a uniform rectangular grid. To synthesize such amplitude masks by the Nanotech SWHL group, a software package was developed, with the help of which masks were designed for obtaining test images with subwavelength resolution. The produced holographic masks were illuminated on an experimental optical table, qualitative images were recorded on a CMOS matrix, and also in the form of prints in a photoresist, including on nonplanar surfaces [4].

The developed software for the holographic mask synthesis is based on the Huygens-Kirchhoff diffraction model. The Huygens-Kirchhoff principle allows one to reduce diffraction problems to
calculation of the interference of waves emitted by secondary sources. This method is well suited for calculating diffraction at sufficiently large in comparison with wavelength openings in opaque thin screens. The disadvantage is its approximate nature and low reliability in the case of openings of small sizes close to the wavelength. Requirement of a large elements size leads to large holographic mask sizes. A study of applicability limits of the Huygens-Kirchhoff principle is an actual goal. The complexity of the problem is due to a large number of parameters of the diffraction problem, such as the curvature of the interface of media with different electrical and magnetic permeability, the screen thickness, the angle of wave incidence. To solve some urgent problems, new approaches to the calculation of diffraction phenomena are required [5-7].

Another factor affecting magnitude of the amplitude holographic mask is the presence of parasitic diffraction orders near the reconstructed field, zero order of diffraction, as an example. To reduce the effect of zero diffraction order on the quality of the useful image, it is necessary to spatially separate the image from the focus of the restoring wave. This is only possible with an appropriate mask size magnification.

In this paper, some variations of holographic mask architecture are proposed, which allow to eliminate the influence of parasitic diffraction orders and reduce the ratio between the mask size and the corresponding image size.

2. Types of holographic mask

Holographic mask is a physical realization of the local amplitude modulation function of the light wave passing through the mask. This function can be obtained as the intensity of reference and object waves interference pattern [3, 8]. The simplest design of the holographic mask is an opaque screen with openings, where the necessary function of local amplitude attenuation is approximated with the density and size of the openings. Elements on such mask should be large enough. It is also necessary to take into account that obtaining high-resolution light images with elements of subwavelength size is possible only with a high angular aperture of the illuminator. Large angles of incidence of the restoring wave and the complex multilayer structure of the mask require to develop an appropriate model of diffraction, which takes into account effects of re-reflection at the layers boundaries, waveguide effects in openings. We will describe the types of holograms with different structures and point to their features and advantages.

2.1. Amplitude hologram

The Gabor’s method of hologram generation is associated with the registration of interference of mutually coherent reference and object waves. Let \((\xi, \eta)\) are coordinates on the hologram plane, \(O(\xi, \eta)\) is the complex amplitude of reference wave on hologram plane, \(\Pi(\xi, \eta)\) is the complex amplitude of object wave. Then, the function

\[
T(\xi, \eta) = \frac{|O(\xi, \eta) + \Pi(\xi, \eta)|^2}{|O(\xi, \eta)|^2},
\]

which takes only non-negative values, will be considered as the function of transmission for amplitude hologram. Note that

\[
T(\xi, \eta)O^*(\xi, \eta) = \frac{|O(\xi, \eta)|^2 + |\Pi(\xi, \eta)|^2 + \Pi^*(\xi, \eta)O^*(\xi, \eta) + \Pi(\xi, \eta)|O^*(\xi, \eta)|^2}{|O(\xi, \eta)|^2} + \Pi^*(\xi, \eta).
\]

Thus, if we highlight the plate with the transmission function \(T(\xi, \eta)\) by the restoring wave \(O^*(\xi, \eta)\), which is a reversed reference wave, the resulting wave in the near field of plate can be decomposed into three components:

- \(\Pi^*(\xi, \eta)\) is the field conjugated to the object wave and focuses in the object image at the object plane;
• \(\left|O(\xi, \eta)\right|^2 + \left|\Pi(\xi, \eta)\right|^2\) is the zero order of diffraction, which in the case of a spherical reference wave and square holographic mask focuses into a bright cross image, which is the diffraction at the edges of the square mask;

• \(\left|\Pi(\xi, \eta)\right|^2\) is the wave field, which focuses into a symmetrical with respect to the focus of the restoring wave, but somewhat distorted, object image.

It is necessary to notice that for possibility of physical realization of the hologram it is required that the coefficient of amplitude modulation does not exceed one in each point. Therefore, making the normalization will receive

\[
T(\xi, \eta) = \frac{|O(\xi, \eta)|^2 + |\Pi(\xi, \eta)|^2}{M * |O(\xi, \eta)|^2},
\]

where \(M = \max\left\{|O(\xi, \eta)|^2 + |\Pi(\xi, \eta)|^2 / |O(\xi, \eta)|^2\right\}\) is a constant value.

Realization of this transmission function is a quartz plate with a thin opaque chromium layer and a set of openings in it, the density and size of which corresponds to the transmission function.

2.2. Amplitude hologram with phase-shifting layer

The zero order of diffraction concentrates most of the restoring wave energy, therefore, interfering with the useful image, it creates significant disturbances. To eliminate a component that corresponds to the zero order, the corresponding real valued term must be subtracted from the transmission function. Then the function

\[
T_1(\xi, \eta) = \frac{|O + \Pi|^2 - (|O|^2 + |\Pi|^2)}{M_1 * |O|^2} = \frac{O' \Pi + O \Pi^*}{M_1 * |O|^2}
\]

takes values from the interval \([-1; 1]\] by selecting a normalization factor \(M_1\) similar to the coefficient \(M\) in the previous case. Modulation of a wave by a negative factor means proportional change of its amplitude and shift of its phase by half of wavelength. Therefore, such transmission function can be implemented physically by applying an additional phase-shifting layer at points with negative modulation.

Note that in this case there is a gain in the diffraction efficiency of the hologram. This is a consequence of inequality

\[
M_1 = \max\left\{\frac{|O' \Pi + O \Pi^*|}{|O|^2}\right\} < M = \max\left\{\frac{|O + \Pi|^2}{|O|^2}\right\},
\]

which is a consequence of triangle inequality. With the right choice of reference wave, the diffraction efficiency is increased by about five times compared to the amplitude mask. This effect is confirmed by numerical experiments.

2.3. Hologram with dimming layers

One of the possible problems of holographic image creation is the lack of light transmission by small openings. On a holographic mask with phase-shifting layer there are quite a lot of such small openings. As shown by previous studies based on the Kirchhoff approximation, on a holographic mask whose dimensions are about 5 times larger than the image size, the vast majority of the transmission zones are in the range \([0; 0.7\lambda]\). In addition to that, mask elements with characteristic dimensions less than \(1.7\lambda\) in a layer of chromium with a thickness of about \(0.5\lambda\) exhibit waveguide properties. This leads to the fact that the calculation of the diffraction on mask elements with sizes in the range \([0.7\lambda; 1.7\lambda]\) is complex, and, taking into account errors of mask manufacturing, is unreliable. During
the passage through the waveguide, the wave is divided into modes that propagate in different
directions (dispersion), that modes fade when moving along the waveguide with different decrement,
reflect differently from the open ends of the waveguide, transmit energy to each other in the presence
of local irregularities within the waveguide and also due to the finite conductivity of the waveguide
material. Thus, the use of elements whose size is less than $1.7\lambda$, on the mask, which is calculated and
optimized in the framework of Kirchhoff's theory, is undesirable.

In order to increase the range of used elements size, it is necessary to significantly increase the
maximum size of the transmission zone, and hence the size of the hologram. The idea of using a
darkening layer is to replace small openings with larger ones with a filtering layer that reduces the
final transmittance. Thus, it is possible to deduce the size of small transmission zones from the
undesirable range and thus save a significant part of the information on the mask. You can go further
and allow the use of multiple dimming layers with different absorption factors.

To calculate the thickness, refractive indices and absorption of phase-shifting and additional
darkening layers, a diffraction model is required, which is fundamentally different from the Huygens-
Kirchhoff formulas. It is important that the function describing the distribution of optical parameters
of the mask layers may have discontinuities.

3. The problem of diffraction in a layered media
A projection method suitable for solving the problem of passing and refracting of a plane wave
through a medium with variable electrical permeability is proposed. To simplify the problem, we make
assumptions about the cylindrical nature of the electrical permeability distribution function
$\hat{\zeta}(x,y,z) = \xi(x,z)$ along the axis $y$, as well as about its periodicity along the axis $x$ with a certain
period $a$. Let the complex-valued function $\xi(x,z)$ change when $z \in (0,z_{\max})$ and $\xi(x,z) = 1$ when
$z \in (-z;0] \cup [z_{\max},+\infty)$, the incident plane wave in the region $z < 0$ has the form $u_0 = e^{ik(x \sin \theta + z \cos \theta)}$, $\theta$ is the angle of incidence, $k = \frac{2\pi}{\lambda}$ is the wave number. We will proceed with the system of
Maxwell's equations for an isotropic medium [8,9]:
\[
\text{rot} \vec{H} - \frac{i\omega}{c} \xi \vec{E},
\]
\[
\text{rot} \vec{E} = \frac{i\omega}{c} \mu \vec{H},
\]
\[
div(\mu \vec{H}) = 0,
\]
\[
div(\xi \vec{E}) = 0.
\]

Let's put the magnetic permeability $\mu$ constant and equal to one. Let us also assume that the
incident plane wave is linearly polarized in the direction of the cylindrical axis $y$. The independence
of the electrical permeability distribution function $\xi(x,z)$ from coordinate $y$ allows us to assert that the
polarization of the passing and refracting waves will remain the same as polarization of incident wave,
and, in accordance with this, to simplify the Maxwell system to the partial differential equation from
one component of the corresponding vector.

3.1. The case of $E$-polarization
Suppose that the vector of the electric field is equal to $\vec{E} = (0,E_y,0)$, the vector of the magnetic field,
respectively, $\vec{H} = (H_x,0,H_z)$. Substituting these assumptions into the Maxwell system, we obtain the
Helmholtz equation
\[
\frac{\partial^2}{\partial x^2} E_y + \frac{\partial^2}{\partial z^2} E_y + k^2 \xi E_y = 0,
\]
with varying, periodic along the axis $x$ and possibly discontinuous coefficient $\xi(x,z)$, from which only integrability on the periodicity interval is required.

We will look for a solution in the form of decomposition of flat waves
\[ E_j(x,z) = \sum B_j(z)\Psi_j(x), \]  
where $\Psi_j(x) = \frac{1}{\sqrt{a}} e^{\frac{i2\pi x}{a}}$, $t = ka \sin \theta$. Note that $\Delta \Psi_j + \lambda_j \Psi_j = 0$, $\lambda_j = \left(\frac{t + 2\pi}{a}\right)^2$.

Boundary conditions on the unknown function $B_j(z)$ are based on the radiation conditions [6]:
\[ z \leq 0: B_j = \delta_0 e^{ikz \cos \theta} + R_j e^{-i\gamma_j z}, \quad \gamma_j = \sqrt{k^2 - \lambda_j} \]
\[ z \geq z_{\text{max}}: B_j = T_j e^{i\gamma_j z}, \quad \gamma_j = \sqrt{k^2 - \lambda_j} \]

The number of elements in the sum (1) is determined based on the conditions $k^2 - \lambda_j \geq 0$ or $-\frac{a(1 + \sin \theta)}{\lambda_j} \leq j \leq \frac{a(1-\sin \theta)}{\lambda_j}$.

To obtain system of ordinary differential equations with the required functions $B_j(z)$ it is required to perform integral transformations of the form
\[ \int_0^a \left( \frac{\partial^2}{\partial x^2} E_j + \frac{\partial^2}{\partial z^2} E_j + k^2 \xi E_j \right) \Psi_j' dx = 0. \]

Then we get the following ODE system:
\[ \frac{d^2}{dz^2} B_j + \left(k^2 - \lambda_j\right) B_j + k^2 \sum_{n=-N_1}^{N_1} k_{jn} B_n = 0, \]
where $k_{jn}(z) = \int_0^a \left(\xi(x,z)-1\right) \Psi_j' \Psi_n dx$, $N_1 = \left[\frac{a(1+\sin \theta)}{\lambda}\right]$, $N_2 = \left[\frac{a(1-\sin \theta)}{\lambda}\right]$.

Boundary conditions are written based on the assumption of the direction of the past and reflected waves: $z \leq 0: B_j(z) = \delta_0 e^{ikz \cos \theta} + R_j e^{-i\gamma_j z}$, $z \geq z_{\text{max}}: B_j(z) = T_j e^{i\gamma_j z}$, where $\gamma_j = \sqrt{k^2 - \lambda_j}$, $\delta_0$ is the Kronecker symbol, $R_j$ and $T_j$ are unknown coefficients, in the form of
\[ \left. \frac{d}{dz} B_j + i\gamma_j B_j \right|_{z=0} = 2i\gamma_0 \delta_0^j, \quad \left. \frac{d}{dz} B_j - i\gamma_j B_j \right|_{z=z_{\text{max}}} = 0. \]

Making the replacement $B_j = P_j$, lowering the order of equations, we get a system of ODE of the form
\[ \begin{align*}
    p' &= b \\
    b' &= Bp
\end{align*} \]
with boundary conditions
\[ p + i\Gamma b \big|_{z=0} = c, \quad p - i\Gamma b \big|_{z=z_{\text{max}}} = 0, \]
where unknown vector-functions $p = \left(P_{-N_1}, \ldots, P_{N_1}\right)^T$, $b = \left(B_{-N_1}, \ldots, B_{N_1}\right)^T$, vector $c = (0, \ldots, 0, 2i\gamma_0, 0, \ldots, 0)^T$, matrix $B = -k^2 K - \Gamma^2$, matrix $K = \{k_{jn}\}$, matrix $\Gamma$ is diagonal with elements $\gamma_j$. 

3.2. The case of H-polarization

Suppose that the vector of the magnetic field is \( \mathbf{H} = (0, H_y, 0) \), the vector of the electric field, respectively, \( \mathbf{E} = (E_x, 0, E_z) \). Substituting these assumptions into the Maxwell system, we obtain the equation

\[
\frac{\partial}{\partial x} \left( \frac{1}{\xi} \frac{\partial H_y}{\partial x} \right) + \frac{\partial}{\partial z} \left( \frac{1}{\xi} \frac{\partial H_y}{\partial z} \right) + k^2 H_z = 0
\]

with similar to the previous case conditions on \( \xi(x,z) \). We will also look for a solution in the form of decomposition on flat waves:

\[ H_y(x,z) = \sum B_j(z)\Psi_j(x) . \]

Equation (2) is reduced by means of similar integral transformation to a system of ODE, which is written in matrix form as

\[
(Kb')' - (K - k^2 E)b = 0
\]

where the unknown vector-function \( b \) is defined in the same way as in the previous case, matrix \( K \) consists of elements \( k_{ij} = \int_0^\xi \Psi_j^* \Psi_i^* dx \), matrix \( K = -\Gamma K \Gamma \), matrix \( \Gamma \) is determined in same way as in previous case. The boundary conditions for unknown functions \( B_j(z) \) are determined similarly.

Making replacement \( Kb' = p \), reducing the order of equations, we obtain ODE system in the very similar form:

\[
\begin{cases}
    p^1 = Ab \\
    b^1 = Bp
\end{cases}
\]

where matrix \( A = K^{-1} \), matrix \( B = K - k^2 E \), and the boundary conditions are

\[
p + i\Gamma Kb\bigg|_{z=0} = Kc , p - i\Gamma Kb\bigg|_{z=\text{max}} = 0
\]

As we can see, both cases are reduced to similar boundary value problems.

3.3. Auxiliary Cauchy problems

Let \( \delta_j = (\delta_{N_1}^j, \delta_{N_2}^j, ..., \delta_{N_1}^j)^T \), \( j = -N_1, ..., N_2 \). Auxiliary Cauchy problems:

\[
\begin{cases}
    p^{1,j} = Ab^{1,j} \\
    b^{1,j} = Bp^{1,j} \\
    b^{1,j}\bigg|_{z=0} = \delta_j , p^{1,j}\bigg|_{z=0} = 0
\end{cases}
\]

\[
\begin{cases}
    p^{2,j} = Ab^{2,j} \\
    b^{2,j} = Bp^{2,j} \\
    b^{2,j}\bigg|_{z=0} = 0 , p^{2,j}\bigg|_{z=0} = \delta_j
\end{cases}
\]

To solve problems of type (1,j) and (2,j), a numerical scheme of the third order of accuracy is used.

That is, the problem in the form (3) with boundary conditions \( b\bigg|_{z=0} = b_0, p\bigg|_{z=0} = p_0 \) is solved according to the scheme

\[
p_{j+1} = p_j + \frac{A^j + A^{j+1}}{2} b_j h + \frac{1}{2} A^j B^j p_j h^2,
\]
\[ b_{j+1} = b_j + \frac{1}{2} (B^{j+1} p_{j+1} + B^j p_j) h, \]

where \( h = \frac{z_{\text{max}}}{N} \), \( N \) is the number of subintervals of interval \([0; z_{\text{max}}]\) partition, \( b_n = b(hn) \), \( p_n = p(hn) \), \( A^n = A(hn) \), \( B^n = B(hn) \), \( n = 0, 1, ..., N \).

3.4. Solution of the diffraction problem

Solution of the problem described by the system (3) with boundary conditions (4) is obtained in the form of a linear combination of solutions of auxiliary problems of types \((1, j)\) and \((2, j)\). Exactly,

\[ b = \sum_{j=-N_1}^{N_1} \alpha_j b^{1, j} + \sum_{j=-N_1}^{N_1} \beta_j b^{2, j}, \]

\[ p = \sum_{j=-N_1}^{N_1} \alpha_j p^{1, j} + \sum_{j=-N_1}^{N_1} \beta_j p^{2, j}, \]

where \( \alpha = (\alpha_{N_1}, \alpha_{N_2-1}, ..., \alpha_{-N_1})^T \), \( \beta = (\beta_{N_1}, \beta_{N_2-1}, ..., \beta_{-N_1})^T \) a unknown vectors that need to be determined. We express vector \( \beta \) from the first boundary condition (4), which in the notations of the previous paragraph can be written as \( p_0 + i K_0 \Gamma b_0 = K_0 c \). Then,

\[ \beta = K_0 (c - i \Gamma \alpha). \]

We will write system for the vector \( \alpha \) basing on the second boundary condition (4). This requires matrices composed of solutions of auxiliary problems \((1, j)\) and \((2, j)\) at the point \( z = z_{\text{max}} \), as of columns. Exactly,

\[ b^i = \begin{pmatrix} b^{i, N_2}_N, b^{i, N_2-1}_N, ..., b^{i, -N_1}_N \end{pmatrix}, \quad p^i = \begin{pmatrix} p^{i, N_2}_N, p^{i, N_2-1}_N, ..., p^{i, -N_1}_N \end{pmatrix}, \quad i \in \{1; 2\}. \]

System of equations for coefficients \( \alpha \) is as follows:

\[ (p^i - (ip^2 K_0 + i K_0 b^i + K_0 \Gamma b^2 K_0 \Gamma) \alpha = (i K_0 \Gamma b^2 - p^2) K_0 c. \]

4. Numerical results

For the numerical experimentations for each of the polarizations software based on Python was developed. Input data for software consist of distribution function of the electrical permeability of the layer, the angle of incidence of the wave, partition parameters. As the output, we obtain the decomposition of the past and reflected waves by plane components, the distribution of the phase and amplitude of the passed wave in the near zone, and the percentage of the past, reflected and absorbed energy. Software interface is shown on the figure 1.

It should be noted that in the case of E-polarization the problem of electromagnetic wave diffraction is identical to the problem of acoustic wave diffraction. This problem was considered in [10], the method of local perturbations was proposed, the accuracy of which in the case of the impedance boundary conditions depends on the small slope and curvature of the interface of the media. To compare the results obtained by the method described in this paper and the method of local perturbations, a series of calculations was carried out, in which the diffraction on the interface between two media was modelled. The proportion of energy absorbed in the medium was calculated and compared for different amplitudes of the relief of the medium and the angles of wave incidence. Figure 2 shows the dependence of the absorbed wave energy proportion \( d \), deposited along the vertical axis, from the amplitude \( A \) of the perturbation of the surface, as a result of diffraction on the surface of the medium. The surface is described by the function \( f(z) = A \sin(z) \), the angle of incidence of the plane wave 30 degrees. Solid line shows the result of the calculation by the method of local variations for the impedance boundary conditions, dotted line shows the results of the calculation by the method described in this paper.
Figure 3 shows comparison of the results of modelling the diffraction on the wavy surface of the media by the method of local variations and projection method. The graph shows the level of dependence of the mutual error $e(\alpha, A) = \left| \frac{d_1-d_2}{d_2} \right| \times 100$ from the angle of wave incidence $\alpha$ and the vertical wave amplitude of the surface $A$.

With the help of the developed software it is possible to observe such known physical effects as Brewster's angle (figure 4) and Wood's anomaly (figure 5).
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Figure 4. The results of the calculation of the reflection of a plane $H$-polarized wave at the plane interface. Angle of plane wave incidence values are plotted on horizontal axis, the percentage of reflected energy values are plotted on the vertical axis. The minimum of energy reflected is achieved when the value of the incidence angle is about 84°.

Calculations of interference mirrors consisting of several dielectrics layers of variable thickness were carried out. A mirror of 6 layers with a reflection coefficient of 86 and a mirror of 8 layers with a reflection coefficient of 95% is obtained by the method of local variations of the layer thickness. This reflection coefficients are preserved at the angle of incidence up to 50°.

Figure 5. Example of diffraction on a wavy structure. Most of the energy of the reflected wave propagates along the surface, subject to certain ratios between the wavelength and the surface wave period.

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