Implementation of the coupled-wave method for V-shaped groove characterization with a scanning differential heterodyne microscope

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Abstract. The image formation theory is presented for scanning differential heterodyne microscope respect to triangular-shaped grooves used for plasmon-polariton waveguiding. The scattering problem of the illuminating probe beams focused on the object surface is resolved with rigorous coupled-wave analysis (RCWA) for groove corrugated grating etched in a substrate with the finite conductivity. To adapt the RCWA method for SDHM the problems were considered associated with a discretization of the diffracted field and sampling the focused probe beams. The focused beams are expanded in terms of plane waves so that the each chosen incident wave is order of one another and then the diffraction problem is solved for every plane wave of TE polarization. The groove was decomposed into thin layers in which the permittivity and electromagnetic field are expanded in Fourier series. The diffraction of the probe beams by triangular groove was analyzed, at that the convergence of modulus and phase responses of SDHM in dependence of the number of the layers and the number of Fourier modes in optical field expansion was investigated. The elaborated algorithm was used for the simulation of differential responses from triangular grooves with various parameters.

1. Introduction

One of directions of development of integrated optics is information transfer with the plasmon-polariton waveguides [1] permitting to achieve the large integration scale of optical circuits. As a rule such waveguides represent etched in metal (usually in gold) submicron grooves with a lamellar or triangular profile [2]. Since characteristics of such waveguides are sensitive to their profile, metrology of these structures is of particular importance. A scanning differential heterodyne microscope (SDHM) due to its common-path configuration providing immunity to vibrations [3] is a promising tool for characterization of narrow microgrooves.

The aim of the work is a development of the SDHM image formation algorithm based on the rigorous coupled-wave analysis (RCWA) [4,5] for simulation of differential responses from triangular grooves. The elaborated method used for calculation of microscope response to V-shaped grooves with various depth and width is need next for characterization V-shaped waveguides by using the experimental responses of the SDHM.

Image formation in the SDHM includes three main stages: (1) diffraction of probe beam by the object surface; (2) transformation of the diffraction field from object plane to a photodetector plane; and (3) formation of a detector signal as a result of an interference of two beams at different frequency.
At the first stage of modeling the microscope response, the scattering of the field of the probe beam from the surface of a microobject must be calculated. In the case of shallow \((h < \lambda/4)\) and broad \((h > \lambda)\) grooves, the scalar theory of scattering can be applied [6]. However, in our case of narrow and deep grooves, one should expect correct results if the rigorous theory is used. Vector methods for solving diffraction problems have been widely used in modern far-field microscopy, which is caused by a decrease in the size of objects under investigation and by increased possibilities for computer processing of images. Both integral [7] and differential [8] methods can be used in this case. However, the former are more suitable for problems that deal with shallow and non-rectangular structures, whereas the latter can be most successfully applied to objects whose profile is rectangular and where the field inside the object can be expanded into orthogonal modes. To solve the diffraction problem for the microscope, we apply the differential RCWA method, which is based on the representation of the field inside the groove as a Fourier expansion. In our model the object under study is a triangular groove etched in metal substrate of a finite conductivity. This object is represented as an element of a one-dimensional periodic grating defined by two parameters: the width \(w\) and the depth \(d\). The period of the grating should be much greater than the size of a focused spot and the width of the groove. Each groove is decomposed into thin layers parallel to object surface, therewith slanted profile of the groove is approximated by piecewise broken line with vertical segments and the permittivity and electromagnetic field in each layer are expanded in Fourier series. Such a representation makes it possible to express the field above the object as a sum of plane waves with different amplitudes. To solve the diffraction problem means to find the expansion coefficients of the field inside and above the groove.

The second and third stages of image formation in the SDHM which will be used in this paper are represented in details elsewhere [9]. In this reference the possibility of factorization of differential response is shown with its representation as a product of two linear ones.

![Figure 1. Geometry for single groove diffraction problem.](image)

2. Image formation theory of SDHM

The optical scheme of SDHM used in modeling corresponds to experimental one and it is based on the Mach–Zehnder interferometer, in which interfering beams travel practically the same path and separate only after focusing on the object. The experimental scheme is presented in detail elsewhere [9]. As a source of linearly polarized light a He-Ne laser \((\lambda = 0.63 \mu m)\) is considered. The object surface is scanned by two closely located focused beams which size are defined by the numerical aperture of the microobjective \(NA = 0.5\) (figure 1). The frequency and spatial separation of the beams is performed by a Bragg cell, interval \(\delta\) between the probing spots can changed by varying the difference frequency of a signal at the cell. The intensity of radiation reflected from the object is detected at difference frequency by a point photodetector located at the center of the Fourier plane of the microscope. The modulus and phase of a harmonic signal of the photodetector form a complex...
response of the microscope during a scanning of the object. Changes in the phase and modulus of probe beams reflected from the object carry information on the profile and structure of the object. The necessary parameters of the object profile could be determined with the appropriate treatment of the response.

To solve diffraction problem with RCWA method we follow reference [4]. The plane wave with wavevector \( \mathbf{k}_0 \) incident at angle \( \theta \) on the periodic 1D grating, with the period \( \Lambda \) exceeding the diameter of focused probe beam, which replaces the isolated groove. First the diffraction on a rectangular grating is considered. The overall space breaks into three regions: over \( (n_1 = 1) \), under \( (n_2) \) and inside grating. The field in each region is defined by the solution of Helmholtz equation as an expansion in terms of eigenmodes in corresponding region. For TE polarization the electric field component \( E_y \) must be satisfied the equation:

\[
\Delta E_y(x,z) + k_0^2 \epsilon(x) E_y(x,z) = 0,
\]

where \( \epsilon(x) \) is relative dielectric permittivity. In the superstrate and substrate, where \( \epsilon(x) = \text{const} \), the solution is given in a simple form as:

\[
E_1^y = E_0 \exp[i(k_0^x x - k_0^z z)] + \sum_{n=-\infty}^{\infty} R_n \exp[i(k_n^x x + k_n^z z)],
\]

\[
E_2^y = \sum_{n=-\infty}^{\infty} T_n \exp[i(k_n^x x - k_n^z z)],
\]

where

\[
k_n^x = k_0 (\sin \theta - n \lambda / \Lambda),
\]

\[
k_n^z = \sqrt{k_0^2 - (k_n^x)^2},
\]

\[
k_{n,1,2}^z = \sqrt{n_1^2 k_0^2 - (k_n^x)^2},
\]

\[
R_n \text{ and } T_n \text{ are the normalized electric-field amplitudes of the } n\text{th backward-diffracted wave (in the superstrate) and forward-diffracted wave (in the substrate), respectively. To solve equation (1) in grating region, the dielectric permittivity } \epsilon(x) \text{ must be expanded in Fourier series of the form:}
\]

\[
\epsilon(x) = \sum_{n=-\infty}^{\infty} \epsilon_n \exp\left\{ \frac{2\pi n x}{\Lambda} \right\},
\]

where \( \epsilon_n \) is the Fourier component of the relative permittivity in the grating region. Then the tangential electric and magnetic fields in grating region may be expressed with a Fourier expansion in terms of space-harmonic fields as

\[
E_n^y = \sum_{n=-\infty}^{\infty} f_n(z) \exp(-ik_n^x x),
\]

\[
H_n^y = -i(\epsilon_0 / \mu_0)^{1/2} \sum_{n=-\infty}^{\infty} g_n(z) \exp(-ik_n^x x),
\]

where \( f_n \) and \( g_n \) are normalized amplitudes of the \( n\)th space-harmonic fields. Substituting equations (4), (5), (6) in the Maxwell's equation one could separate the variables \( z \) and \( x \) and obtain the coupled-wave equations of the form.
\[
\frac{\partial f_n}{\partial z} = k_0 g_n,
\]
\[
\frac{\partial g_n}{\partial z} = \left(\frac{k_0}{k_0} f_n - k_0 \sum_{p=-\infty}^{\infty} g_{n-p} f_n,\right)
\]
which being represented in matrix form are solved by finding the eigenvectors and eigenvalues associated with the characteristic matrix of the equation (7). Matching the tangential electric and magnetic field components at the boundaries one can calculate the amplitude of diffracted fields and find the elements \(R_n\) of the reflection matrix. These coefficients define reflected field
\[
E'_y = \sum_{n=-\infty}^{\infty} R_n \exp\left[i(k_n^z x + k_n^x z)\right]
\]
propagating from object surface to photodetector plane through the optical microscope system.

For grooves of arbitrary profile (including triangular grooves) the grating region is decomposed into thin layers parallel to object surface (figure 2). Then for each layer the eigenvalue problem is resolved by RCWA and the diffraction coefficients \(R_n\) are determined by matching the tangential electromagnetic fields at the boundaries between the grating layers.

**Figure 2.** Geometry for surface-relief grating divided into a large number of thin planar slabs.

As in optical system of SDHM the object is illuminated by focused beam the scattering of focused beam must be considered. To do this we define the incident field in XY-plane as a Fourier transform of beam field distribution in Fourier plane \((q,p)\) and sample the Fourier integral to obtain truncated sum of \((2M+1)^2\) space harmonics as
\[
g(x,y) = \frac{1}{M^2} \sum_{m=-M}^{M} \sum_{l=-M}^{M} \Pi(q_m, p_l) \exp(iq_mx) \exp(ip_ly),
\]
where
\[
\Pi(q_m, p_l) = \begin{cases} 
1, & \text{if } \sqrt{q_m^2 + p_l^2} \leq k_0 \cdot \text{NA} \\
0, & \text{if } \sqrt{q_m^2 + p_l^2} \geq k_0 \cdot \text{NA} 
\end{cases}
\]
is the transfer function of the microobjective, \(q_m = k_0 \cdot \text{NA} \cdot m/M, p_l = k_0 \cdot \text{NA} \cdot l/M\), NA is the numerical aperture of the microobjective. If the point photodetector is located in the center of the Fourier plane
then \( p = 0 \) and any \( \ell \)th space harmonic in equation (9) is not diffracted normally, because the grating vector lies in XZ-plane. Therefore the incident beam can be reduced to 1D approach in the form

\[
g(x, y) = \frac{1}{M} \sum_{m=-M}^{M} \prod(q_m) \exp(iq_m x).
\]  

(10)

The coherent method of signal registration in the center of the Fourier plane allows to increase the discretization interval and reduce the number of space harmonics in equation (10) in numerical computations. In this case the contribution in the response is brought only by components for which \( q_{mn} = q_m - 2\pi n/\Lambda = 0 \). Thus \( M \) is defined as \( M = 2\text{NA}/\Lambda \). It means that for the sampling of the focused beam it is enough to represent it as a set of those plane waves which wave vectors coincide with grating diffraction orders of normally incident plane wave.

Further the diffraction problem is solved for each incident plane wave in equation (10) and the reflected field over the grating is expressed as

\[
E'_y = \sum_{m=-M}^{M} \sum_{n=-\infty}^{\infty} R_{mn} \exp[i(q_{mn} x + \sqrt{k_0^2 - q_{mn}^2} z)],
\]  

(11)

where \( q_{mn} = q_m - 2\pi n/\Lambda \) and \( R_{mn} \) is the diffracted amplitude of the \( n \)th reflected wave for \( m \)th incident wave. This expression is used next for determination of SDHM response.

The optical field in registration plane \((u, v)\) is defined by linear transform of equation (11) as

\[
L(u, v) = \int \int G(u, v, x, y) E'_y \bigg|_{z=0} \ dx \ dy,
\]  

(12)

where \( G \) is the point spread function. If the UV-plane coincides with the Fourier plane, then

\[
G(q, p, x, y) = P(x, y) \exp(-ix) \exp(-ipy),
\]  

(13)

where \( P \) is the pupil function of the microobjective. In the center of the Fourier plane \((q = p = 0)\) we have

\[
L = \frac{2\pi a^2}{M} \sum_{m=-M}^{M} \sum_{n=-\infty}^{\infty} R_{mn} J_1(aq_{mn}) \frac{aq_{mn}}{aq_{mn}},
\]  

(14)

Here \( J_1 \) is the Bessel function of the first kind of zeroth order, \( a = f\text{NA}, f \) is the focal length of the microobjective.

The infinite Fourier expansion (8) should be truncated for numerical calculations. We believe that the computed fields are described with sufficient accuracy by \( 2N + 1 \) Fourier components herewith the choice of \( N \) depends on convergence rate of differential response. Also the convergence properties of microscope response must be determined for the number \( K \) of grating layers. The change of amplitude and phase response in dependence on \( N \) and \( K \) shows that the convergence is fast enough and the accuracy achieves 5%-RMS error of the response (figure 3).

In optical scheme of SDHM object surface is illuminated by two focused beam with different frequencies. Reflected fields interfere in the Fourier plane and induce the photocurrent of point detector at heterodyne (difference) frequency. These features of the optical scheme result to factorization of the function of differential response which is expressed as a product of two linear response in the form

\[
D(x, \delta) = L(x, +\delta/2)L^*(x, -\delta/2).
\]  

(15)

where \( x \) denotes the groove coordinate and \( \delta \) is the interval between focused spots. This expression allows to compute amplitude and phase responses at various object parameters and microscope parameters.
Figure 3. The RMS errors of phase and amplitude response in dependence of the number $K$ of grating slabs and the number $N$ (herewith the number of Fourier harmonics in diffracted field is $2N+1$).

3. Numerical results

We apply algorithm presented for response formation to simulation of differential responses to triangular grooves. As it was mentioned above the groove to be investigated can be represented as an element of periodic grating. The period of this grating must be more than the probe spot’s diameter. The following parameters were used in calculations: the grating period $\Lambda = 5 \mu m$, the groove depth $d$ changes in the range $0.9\div1.1 \mu m$, the groove width $w = 0.4 \mu m$ and $0.5 \mu m$, the refractive index of the substrate $n_2 = 0.16 + 3.9i$. The spot diameter of probe beam was determined as $\lambda/2NA = 0.6 \mu m$ (for wavelength $\lambda = 0.63 \mu m$ and NA = 0.5). The interval between probing spots is $\delta = 0.2 \mu m$.

Figure 4. Simulated phase and amplitude responses to triangular groove with width $w = 0.4 \mu m$ (a,b), $w = 0.5 \mu m$ (c,d) and depth $d = 0.9$ (curve 1), 1.0 (curve 2), 0.6 $\mu m$ (curve 3) for TE polarization.
The phase and amplitude responses to triangular groove at various depths and two widths are presented in figure 4 for TE polarization. As the phase images of the groove appear as differential curves which magnitudes depend on groove parameters the magnitude of response (denoted as contrast) could characterize groove depth and width. One should take into account the sign of differential response which is identified with the polarity of first pulse in phase response. For example, the phase responses presented in figure 4(a) have a negative contrast and responses in figure 4(c) acquire the positive contrast. Such designation is important for introducing later notation of phase contrast which is needed for characterization of V-shaped grooves according to experimental responses of the SDHM. As follows from figure 4 the change of groove depth and width varies both the amplitude and phase response. One can see the high sensitivity of microscope responses (phase and amplitude) to changing grooves parameters $w$ and $d$. Taking into account the real microscope noise we have estimated the sensitivity as $\Delta d = 0.02 \mu m$ and $\Delta w = 0.01 \mu m$.

4. Conclusion

An algorithm is elaborated for numerical calculation of TE-response of the SDHM to deep narrow grooves of arbitrary profile. The complex differential responses from triangular microgrooves are calculated for various depth and width. The RCWA approach yields a stable numerical solution of the diffraction problem for triangular microgroove illuminated by SDHM probe beam at TE polarization. The phase and amplitude response of SDHM in dependence on the number of Fourier harmonics $2N + 1$ in field expansion and the number $K$ of approximating segments of object profile has shown that both phase and amplitude responses converge to the proper values if $N$ and $K$ exceed 70. An optimal sampling of focused probe beam at the coherent signal registration in Fourier plane is realized when space harmonics propagate in directions of diffraction orders. Then the probe beam could be sampled by limited number of plane waves ($M = 9$). The elaborated image formation algorithm based on RCWA could be applied for characterization with high sensitivity of V-shaped groove used as waveguides for plasmon polaritons.

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