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Application of an approximate vectorial diffraction model to analysing diffractive micro-optical elements*

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Scalar diffraction theory, although simple and efficient, is too rough for analysing diffractive micro-optical elements. Rigorous vectorial diffraction theory requires extensive numerical efforts, and is not a convenient design tool. In this paper we employ a simple approximate vectorial diffraction model which combines the principle of the scalar diffraction theory with an approximate local field model to analyse the diffraction of optical waves by some typical two-dimensional diffractive micro-optical elements. The TE and TM polarization modes are both considered. We have found that the approximate vectorial diffraction model can agree much better with the rigorous electromagnetic simulation results than the scalar diffraction theory for these micro-optical elements.

Keywords: approximate vectorial diffraction theory, micro-optical diffractive elements
PACC: 4225B, 4225F, 4225G

1. Introduction

Scalar diffraction theory (SDT) has been widely employed to understand and predict the propagation properties of a light beam through diffractive optical elements (DOEs).[1−3] Physically founded on the Huygens–Fresnel principle and mathematically based on the Kirchhoff formula, this model is conceptually elegant and numerically friendly. Nevertheless, numerous experiences have shown that when the characteristic scale of the microstructure of the DOE is comparable with the wavelength of the incident light, the SDT becomes inadequate qualitatively and inaccurate quantitatively.[4] In this situation, vectorial diffraction theory (VDT) should be adopted. Based on rigorous electromagnetic analysis (virtually Maxwell equations), the VDT requires extensive and expensive numerical efforts, and the burden increases rapidly with the size of the DOE.[5−10] Therefore, a quantitatively accurate and numerically friendly model is highly desired. Recently, Tururen and his co-workers analysed the disturbance of electromagnetic fields by abrupt surface-profile transitions of DOEs from the prediction by the conventional thin-film approximation model. Thereby, they incorporated a more accurate disturbed optical field around the transition edge into the scalar diffraction theory, and improved the result for non-paraxial DOE.[11,12]

In this work, following the similar physical principle, we present an approximate model which combines the merits of the SDT and VDT and apply it to solving the diffraction problem of electromagnetic waves by two-dimensional (2D) micro-optical diffractive elements. In order to see the essentials of the proposed model, let us first revisit the principle of the SDT. The diffraction optical field $U(\boldsymbol{r})$ at a given observation point $\boldsymbol{r}$ is related to the near-field $V(\boldsymbol{r})$ at the exit surface S of the DOE by the well-known Kirchhoff formula

$$U(\boldsymbol{r}) = \int_S G(\boldsymbol{r}, \boldsymbol{r}')V(\boldsymbol{r}')\mathrm{d}S', \qquad (1)$$

where $G(\boldsymbol{r}, \boldsymbol{r}')$ is a propagation operator. In the SDT, a significant approximation has been made, where

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$V(\boldsymbol{r}) = V_s(\boldsymbol{r})$ is assumed to have a very simple and elegant relation with the incident field $V_0(\boldsymbol{r})$. In the case of an open aperture, $V_s(\boldsymbol{r}) = V_0(\boldsymbol{r})$ inside the aperture, and $V_s(\boldsymbol{r}) = 0$ outside the aperture. In the DOE case, the thin-film approximation is adopted, where $V_s(\mathbf{r}) = tV_0(\boldsymbol{r})\exp[\mathrm{i}\phi(\boldsymbol{r})]$. Here t is the transmission coefficient, and $\phi(\boldsymbol{r})$ is the local phase-shift of the DOE. As V is the optical near-field of the DOE microstructure, the simple phase-shift picture is problematic, especially at the discontinuity edge of two adjacent phase-domains. Due to strong scattering effect, the real near-field V can significantly deviate from V_s. However, the thin-film model is accurate in the region sufficiently far from the edge. So it is understandable that for a macroscopic DOE with the minimum phase-domain size far larger than the wavelength, the SDT remains very accurate because the edge region only occupies a very small fraction of the whole DOE. However, the approximation will become bad for a micro-optic element since the edge region can play a dominant role.

From the above physical picture it is clear that the key to a superior model over the SDT is to adopt the correct optical near-field distribution $V(\boldsymbol{r})$, at least in the edge regions. To this end, we employ a local perturbation model (called the approximate vectorial diffraction theory (AVDT)) where the near-field around the phase-domain edge is calculated as if there existed only one abrupt phase-domain edge, and couplings among different domain edges are neglected. This near-field can be simulated by investigating a grating with a sufficiently large period and the same phase-shift by means of a rigorous coupled-wave theory [13,14] or a more general transfer-matrix method.[15,16] Then as a first-order approximation, the calculated field around the edge is recorded and inserted into Eq.(1), serving as $V(\boldsymbol{r})$. As the global coupling effect of the whole DOE has been neglected, the huge numerical burden associated with a rigorous VDT is avoided.

In the classical diffraction theory, the propagation operator $G(\boldsymbol{r}, \boldsymbol{r}')$ in Eq.(1) can have different forms, depending on the boundary condition of the fields and Green's function[1] used. There are several kinds of traditional boundary conditions, such as the Kirchhoff boundary condition, Dirichlet boundary condition, and Neumann boundary condition. In the AVDT, only the optical near-field distribution $V(\boldsymbol{r})$ is considered and solved by means of the rigorous grating theory, while the normal derivative of the near-field is neglected for simplicity. Of course, the normal derivative can also be solved by the rigorous grating theory, however, it will add much complexity to our approximate diffraction model, but no much improvement can be brought to the accuracy of the approximate model. In this situation, we choose the Dirichlet boundary condition and only consider the optical near-field in the formulation of Eq.(1). The Dirichlet boundary condition can be combined with Huygen's principle and the appropriate Green function to obtain the Rayleigh–Sommerfeld diffraction integral of the first kind.[1] Then the propagation operator $G(\boldsymbol{r}, \boldsymbol{r}')$ can be given by

$$G(\boldsymbol{r}, \boldsymbol{r}') = \frac{\mathrm{i}kz}{2|\boldsymbol{r} - \boldsymbol{r}'|} H_1^{(2)}(k|\boldsymbol{r} - \boldsymbol{r}'|). \qquad (2)$$

Here k represents the wave number of the incident light, and z is the projection length of the vector $\boldsymbol{r} - \boldsymbol{r}'$ on the propagation axis. $H_1^{(2)}$ denotes the first-order Hankel function of the second kind.

After knowing $V(\boldsymbol{r}')$ and $G(\boldsymbol{r}, \boldsymbol{r}')$, the diffractive field in any plane behind a DOE can be determined by Eq.(1). To see whether the proposed model AVDT can work well, in the next section we will compare a set of computational results of the diffractive field by means of the SDT, AVDT and VDT about several typical 2D DOEs.

2. Simulation results for diffractive micro-optical elements by using different diffraction models

We first examine a simple 2D micro-optical DOE as schematically shown in Fig.1(a). We first consider the situation where the incident light is in a TE polarization mode: namely, the electric field is parallel to the homogeneous direction of the DOE and thus $\boldsymbol{E} = E_y\hat{y}$. The DOE is a 2D lamellar grating built in to a glass substrate but with a finite number (five) of period. The substrate surface outside the grating is black. The period of the grating is 4μm, the glass and air domains each are 2 μm wide, and each groove is 1.1 μm deep. The incident wave (at a wavelength λ=633nm) impinges upon the DOE from the glass substrate, and is diffracted by the grating. We first carry out calculation by using the SDT. The diffraction field pattern in an observation plane 40 μm away from the surface of the grating is displayed in Fig.1(b) by the dashed line. The calculated diffraction pat-

tern overall shows an apparent oscillation-decay profile. Among the four dominant peaks, the central two peaks are remarkably higher than the other two. This result is in accordance with a simple physical picture expected from the SDT, where the diffraction field should originate from two dominant effects: one is the diffraction by the open aperture (20μm wide), and the other is the interference effect from the five identical phase-domains. Next we perform the same numerical simulation by means of the AVDT. The result is shown in Fig. 1(b) by the solid line. The interference effect is still very apparent, similar to the SDT result. However, the central four dominant peaks are almost identical in strength, but significantly different from the SDT diffraction pattern. This seems to indicate that the diffraction effect from the open aperture is shadowed by other complex scattering effects for this micro-optical element. To see which method can really reflect the physical essence, we employ a rigorous electromagnetic technique called boundary element method (BEM)[5−8] to make the same calculation. The result is displayed by the dotted line in Fig.1(b). Evidently the AVDT gives the result in excellent agreement with the rigorous result, while the SDT yields too rough a prediction on the diffraction behaviour of light by this micro-optical element. To make a quantitative comparison between three results, we define a relative difference parameter ΔA_{ab} as the ratio of the absolute difference between the intensity value of the diffractive field by the AVDT and the intensity value by the BEM to the absolute intensity value by the BEM, and ΔA_{sb} as the ratio of the absolute difference between the intensity value by the SDT and intensity value by the BEM to the absolute intensity value by the BEM. We obtain $\Delta A_{ab} = 0.84\%$ at two central peaks, much less than $\Delta A_{sb} = 22.13\%$. Moreover, comparing with the rigorous electromagnetic method, the AVDT has an advantage of less computing time. In this case, the three results are all obtained by use of a computer with CPU 800 MHz and 256M Memory. The computing time taken by the BEM is about 7500 seconds, being 750 times the time (10 seconds) taken by the AVDT. Therefore, the proposed AVDT is expected to obtain more accurate result than the SDT in very little computing time comparing with the BEM.

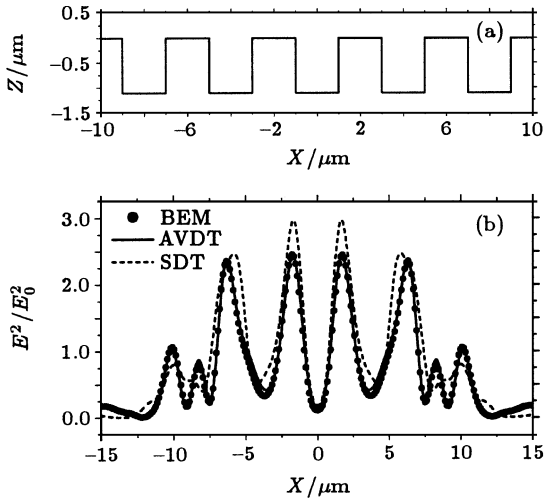


Fig.1. (a) Schematic geometry of the surface-relief grating. Note that the y-axis is perpendicular to the page and points inside. (b) Diffraction E_y field patterns by a finite-number-of-period grating by means of the SDT, the AVDT, and the BEM, respectively. The incident wave is in the TE polarization mode.

Next we turn to a more common micro-optical DOE, a 2D diffractive microlens built into a glass substrate. The lens is 42μm wide, and the presumed focus length is 40μm, corresponding to an f-number of about 1. The lens has been 8-level quantized and each pixel is 2μm wide. Note that this is not a standard way to quantize a diffractive lens. The geometrical configuration of the resulting surface-relief structure is schematically depicted in Fig.2(a). We have used the SDT and AVDT to investigate the diffraction optical field for a normally incident planar wave ($\lambda = 633$nm) from the substrate, and the calculated diffraction patterns of the E_y field in the focal plane are displayed in Fig.2(b) by the dashed and solid lines, respectively. Also, in order to judge to what extent the two approaches are in agreement with each other, we carry out the BEM simulation and the result is shown by the dotted line in Fig.2(b). Obviously, the AVDT also gives the result in much better agreement with that from the BEM than the SDT. We obtain $\Delta A_{ab} = 1.31\%$ and $\Delta A_{sb} = 9.22\%$ at a central peak. Although these results are rough, the SDT still predicts a qualitatively correct focusing behaviour. In this regard, the SDT can still play an important role in analysing such kinds of micro-optical elements.

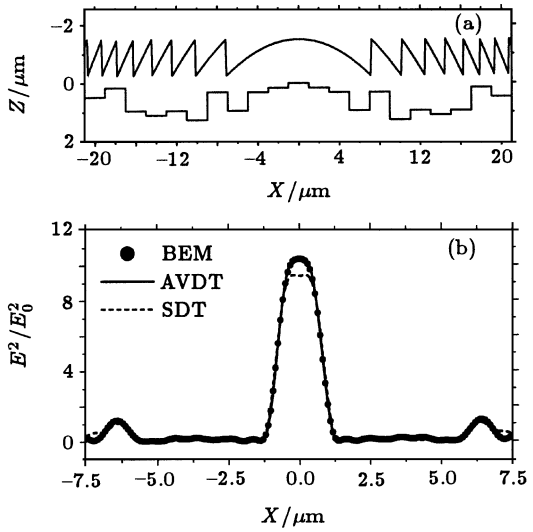


Fig.2. (a) Schematic geometry of the surface-relief structure with continuous phase distribution (upper panel) and 8-level quantized phase distribution, each pixel of which is 2μm wide (lower panel). The y-axis is perpendicular to the page and points inside. (b) Calculated diffraction E_y field patterns in the presumed focal plane by an 8-level quantized diffractive microlens.

In the above two micro-optical elements, the subtle microstructure (namely, each pixel) has a minimum size of 2μm, about 3 times the wavelength. Since the optical near-field around the phase-domain edge only remarkably deviates from the distribution predicted by the SDT in a region of about 1.5 λ on each side, the perturbation due to radiation from other phase domains (namely, the global coupling effect) can be safely neglected in these structures. Therefore, the AVDT can be very accurate in predicting the optical properties of these micro-optical elements. Naturally, when the DOE is dominantly composed of subwavelength microstructures, the AVDT will become less accurate, and even incorrect, because the basis on which the local perturbation approximation is developed no longer stands due to more and more significant coupling effects between different phase-domains.

Keeping this in mind, we consider another 2D diffractive microlens, which has a presumed focus length of 40μm, an f-number of 1. The continuous phase distribution of this lens is schematically shown in the upper panel of Fig.3(a). It can be found that the width of each phase-domain becomes narrower and narrower, i.e. farther and farther from the lens axis, until it becomes much smaller than the wavelength. We select a 30μm wide diffraction aperture for the lens, and consider a binary quantization over the continuous phase distribution. The geometry of the resulting surface-relief structure is displayed in the lower panel of Fig.3(a). The narrowing trend of the phase-domain is obvious. We also carry out SDT and AVDT simulations of the optical field in the focal plane for the TE polarization mode, and check the results by means of the BEM. Figure 3(b) shows the field patterns in a window around the presumed focal point, calculated by means of the three models. It can be seen that the SDT and AVDT are both fairly satisfactory in predicting the basic focusing behaviour of the microlens compared with the rigorous BEM. On the other hand, the SDT presents the result in better agreement with that from the BEM than the AVDT. This is different from the above two micro-optical elements. The reason for that can be understood by noticing that at the outermost edge of the lens the phase-domain can be as narrow as 0.2 μm. The near-field in these domains will strongly deviate from what is predicted by the AVDT, and as a result will contribute significant inaccuracy to the total diffraction field. This example clearly reveals the extent to which

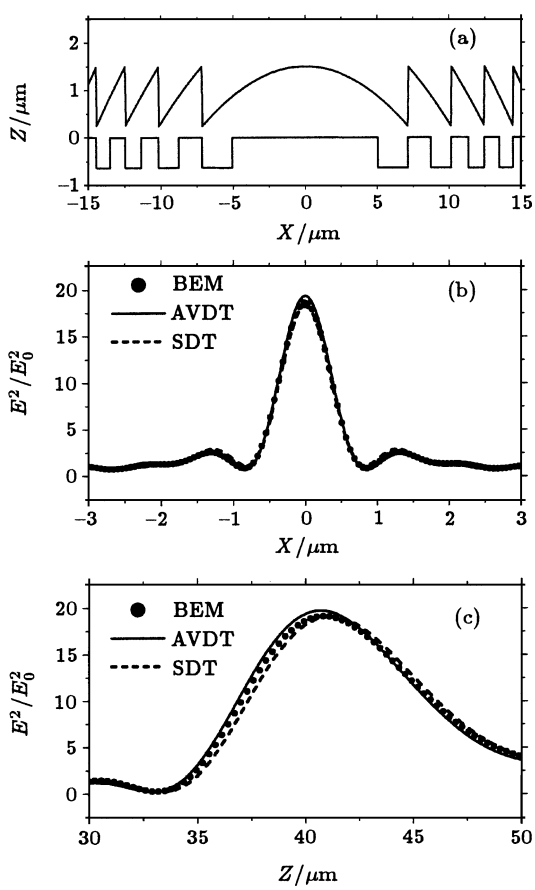


Fig.3. (a) Schematic geometry of the surface-relief structure with continuous (upper panel) and binary (lower panel) phase distribution. The y-axis is perpendicular to the page and points inside. (b) Calculated diffraction E_y field patterns in the presumed focal plane and along the axial direction (c) of a binary diffractive microlens.

the AVDT is valid. When we look into the field pattern along the optical axis of the lens, we observe that the AVDT can still predict more correct focal length than the SDT. Figure 3(c) shows the field patterns in a window around the presumed focal point, calculated by means of the three models. The AVDT and BEM both yield a focal point 40.8μm away from the surface of the lens, while the SDT predicts a focal length of 41.1μm, and the pattern overall shifts towards the real one.

The above three examples all correspond to the TE polarization of electromagnetic field, i.e. the polarization direction of the electric field components of the incident optical wave is parallel to the extending orientation of the grooves of 2D micro-optical DOE. We have also investigated the diffraction of an incident optical wave in the TM polarization mode by the above-mentioned three micro-optical elements. In the TM polarization mode, the polarization direction of the magnetic field component is along the extension direction of the grooves of the 2D micro-optical DOE. In this situation we have $\boldsymbol{H} = H_y\hat{y}$.

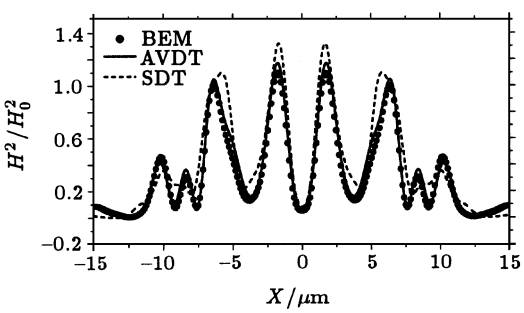


Fig.4. Diffraction H_y field patterns by a finite-number-of-period grating by means of the SDT, the AVDT, and the BEM, respectively. The incident wave is in the TM polarization mode. The schematic geometry of the surface-relief structure is the same as that in Fig.1(a).

The calculated intensity distribution of the diffractive H_y field for an incident planar wave by the first micro-optical DOE is displayed in Fig.4. The solid line represents the result obtained by using the AVDT. The dashed and dotted lines correspond to the results from the SDT and the BEM, respectively. As can be found in Fig.4, in the SDT model, the diffractive field patterns also have four dominant peaks, among which the central two peaks are remarkably higher than the other two peaks. However, in the AVDT model, the central two diffractive peaks become almost identical to the other two peaks, possibly because of the complex scattering effects by the abrupt transition structure of the micro-optical DOE. These features are similar to those in the TE polarization case, as shown in Fig.1(b). By comparing the results from the AVDT and the SDT respectively with the rigorous simulation result obtained by the BEM it can be found that, the accuracy of AVDT prevails over that of the SDT. In this case, $\Delta A_{\rm ab} = 7.01\%$ and $\Delta A_{\rm sb} = 20.48\%$ at two central peaks. Figure 5 corresponds to the intensity distribution of the diffractive H_y field by the second micro-optical DOE, the 8-level quantized micro-optical lens as schematically shown in Fig.2(a). The three curves represent the simulation results by means of the three models: the AVDT, SDT, and BEM, respectively. Similar to the results in Fig.2(a), the rigorous BEM results and the AVDT results each show a central diffractive peak higher than expected by the SDT. We obtain $\Delta A_{ab} = 4.99\%$ and $\Delta A_{sb} = 10.44\%$. On the other hand, the AVDT presents the results whose accuracy in the TM mode is lower than in the TE mode while the rigorous BEM does not give such results as the AVDT, however, the AVDT is still more accurate than the SDT.

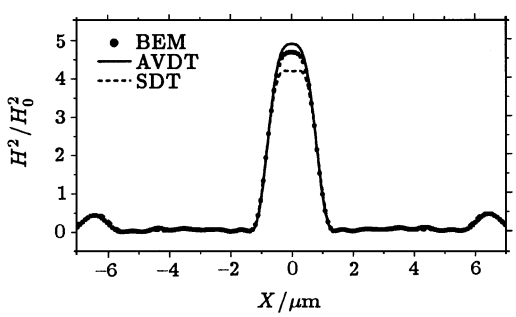


Fig.5. Diffraction H_y field patterns by a 8-level quantized microlens by means of the SDT, the AVDT, and the BEM, respectively. The incident wave is in the TM polarization mode. The schematic geometry of the surface-relief structure is the same as that in Fig.2(a).

Figure 6 shows the intensity distribution of the diffractive H_y field generated by a two-level quantized 2D diffractive microlens, which is the same as that shown in Fig.3(a). The solid, dashed, and dotted lines correspond to the simulation results obtained by means of the AVDT, SDT, and BEM schemes, respectively. Figure 6(a) displays the intensity distribution of the H_y field in the observation plane 40μm away from the surface of the micro-optical DOE, which is the same as that shown in Fig.3(b). We can see that the SDT and AVDT are satisfactory in predicting the basic focusing behaviour of the microlens compared

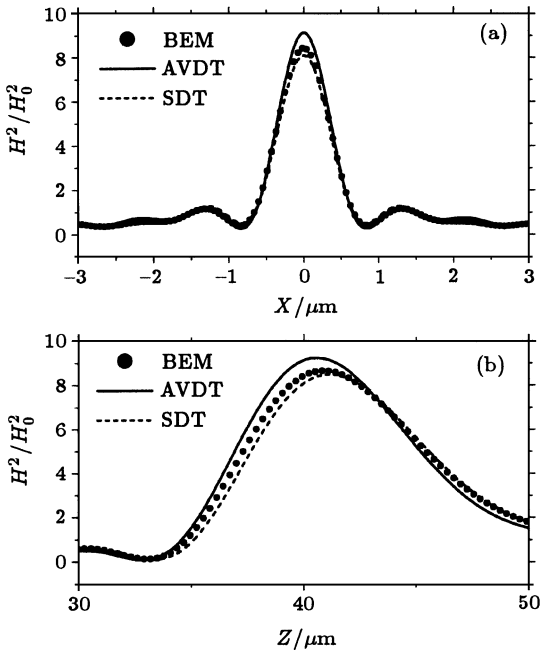


Fig.6. (a) Calculated diffraction H_y field patterns in the presumed focal plane and along the axial direction (b) of a binary diffractive microlens. The schematic geometry of the surface-relief structure is the same as that in Fig.3(a).

with the rigorous BEM. However the SDT gives a result in better agreement with that obtained from the BEM than the AVDT. We also calculate the intensity distribution of the H_y field along the optical axis of the micro-optical lens by using the three methods, and the results are schematically shown in Fig.6(b). The accurate focal point calculated by the rigorous BEM is found to locate in the plane 40.8μm away from the surface of the microlens. The focal lengths predicted by the SDT and the AVDT are 41.1μm and 40.7μm, respectively. Therefore, the AVDT also exhibits a better accuracy than the SDT in predicting the focusing length of a microlens.

3. Conclusion

In summary, we have applied an approximate vectorial diffraction model to analysing the optical properties of diffractive micro-optical elements. This model is physically simple and elegant, numerically friendly, and quantitatively accurate. Application of this approximate model to several typical 2D diffractive micro-optical elements such as a finite-width periodic binary structure and a diffractive microlens respectively under the excitation of the TE and TM polarization modes has revealed an accuracy much better than that obtained from the conventional scalar diffraction theory and the computing time much less than that taken by the rigorous electromagnetic theory. It is expected that this model can be of help to efficient design of micro-optical elements.

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