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Optimal Design and Fabrication of Fine Diffractive Optical Elements Using Proximity Correction with Electron-beam Lithography

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1. Introduction

In recent years, diffractive optical elements (DOEs) are widely used for applications to optical disc pickup, array generators, spectrum filtering, wavelength division multiplexing (WDM), and many others. The DOEs with small feature sizes can be fabricated by the direct-writing electron-beam lithography. (Kley, 1997) To predict the electron dosage to obtain a desired resist profile, the effects of electron scattering in a resist layer and resist characteristics of development process must be considered. (Neureuther et al., 1979) Determining the optimum electron dose is called the proximity correction.

Some methods of the proximity correction were proposed, (Maker & Muller, 1992; Daschner et al., 1995; Nikolajeff et al., 1995) which are classified according to estimation methods of resist profile. One popular method is based on a point-spread function of the electron scatter and a resist contrast curve. (Daschner et al., 1995) The point-spread function is the density distribution of absorbed energy for a focused electron-beam. The function can be assumed to be the sum of two Gaussian distributions due to forward scattering and back scattering. The absorbed energy density is expressed by a convolution of the electron dose distribution and the point-spread function. The resist profile after developing is estimated from the absorbed energy density and a resist contrast curve. The resist contrast curve shows the remaining resist thickness as a function of the absorbed energy density. The point-spread function and the resist contrast curve are determined experimentally. This estimation method is widely used because of the simple process of calculation. However the contrast curve method is not valid for short-period gratings with deep grooves, because the absorbed energy density is not uniform vertically. (Okano et al., 2000) We had reported a precise proximity correction method based on the electron-beam lithography simulator, (Hirai et al., 2000) which consists of an electron scatter simulation by the Monte Carlo method (Kyser & Murata, 1974) and a resist development simulation with the cell removal model. (Dill et al., 1975) This correction method is suitable for short-period gratings and chirped period diffraction gratings such as a diffractive lens. (Okano et al., 2003)

Diffraction efficiencies of the periodic diffraction gratings can be calculated by numerical analysis such as the rigorous coupled wave analysis (RCWA) method, (Moharam & Gaylord, 1981) the differential method, (Vincent, 1980) and the finite difference time domain (FDTD) method. (Yee, 1966) The diffraction efficiency is defined as a ratio of an incident and the

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diffracted beam powers. It is known that when the grating period is several times as long as the light wavelength ($<5\lambda$), the saw teeth profile is not the solution to obtain the highest efficiency of the first order diffracted light.(Shiono et al., 2002) There are some reports to calculate the grating profile to obtain the highest diffraction efficiency using the rigorous grating analysis.(Nojonen et al., 1992; Sheng et al., 1997; Kallioniemi et al., 2000; Testorf & Fiddy, 2001) The diffraction efficiencies of the optimized gratings were taken very high values. Nojonen et al. found the grating profile with the efficiency of 85.7% in case the diffraction grating has a period of 2.5λ .(Nojonen et al., 1992) If the grating profile is the simple saw teeth, the efficiency will be $\sim 45\%$. However, such the short period gratings are not easy to be fabricated with the direct-writing electron-beam lithography, because the optimized grating profiles have sharp peaks and narrow valleys. The proximity effect of electron scattering restricts the grating profiles. A small difference of the grating profile from the designed one causes a decrease of diffraction efficiency.

For chirped-period diffraction gratings, the boundary element(Hirayama et al., 1996) and FDTD(Prather et al., 2001) methods are used for calculating the diffraction efficiency. Prather et al. showed that a multilevel diffractive lens with a small F -number (<1.5) should be analyzed by rigorous electromagnetic wave analysis.(Prather et al., 2001) In some reports, an optimizing design for highly efficient diffractive lenses with a small F -number by simulated quenching(Prather et al., 1998) and Gerchberg-Saxton algorithm(Di et al., 2003) is described. Moreover, a diffractive lens consisting of a subwavelength grating structure is suggested.(Prather et al., 1998) These optical design methods are based on only an electromagnetic analysis without restrictions on fabrication limits; thus, it may be difficult to fabricate the designed grating profile, particularly for short-period gratings.

In this chapter, we demonstrate a unified design method optimizes the electron dose and grating profiles simultaneously to obtain the desired diffraction efficiency under the restriction of the proximity effect.(Okano et al., 2004; 2007) The optimization is made with the rigorous electromagnetic wave analysis and the resist development simulator. We design two cases of short periodic diffraction grating and the diffractive lens using the unified design method.

2. Optimal design method within proximity correction and grating analysis

Figure 1 shows the optimal design flow of the DOEs by the electromagnetic grating analysis and the electron-beam lithography simulation. After assuming the electron dose profile D on the resist layer, the resist profile P is calculated by electron-beam lithography simulation. Then the diffraction efficiency η_i of the resist profile P is calculated by the RCWA or the FDTD method, where the suffix i is the diffraction order. The merit function ϕ is defined as a sum of mean square of the differences ($\eta_i - \eta_i^d$). Here, η_i^d is a desired diffraction efficiency. If the value of merit function ϕ is larger than a certain small value $\Delta\phi$, the exposure dose profile D is modified. These calculations are iterated until the value of the merit function ϕ is less than $\Delta\phi$ or it is converged well. Consequently, we will obtain the optimized grating profile P , the diffraction efficiencies η_i and the electron dose profile D for the fabrication, simultaneously.

This optimal design method searches an optimum grating profile under the restriction of the proximity effect, that is, we find the fabricatable best solution. In the following simulation, we take unity for all of weight W_i . The modified electron-dose profile D is expressed as a polynomial function of 9th-order in each grating period. Therefore the

number of parameters to be optimized is 10. We use the simulated annealing method(Kirkpatrick et al., 1983) as an algorithm of the optimization method.

Several parameters of the electron-beam resist are required for the lithography simulation. The resist parameters must be determined from a primary experiment.(Okano et al., 2003) We used the resist parameters of OEBR-1000 (Tokyo Ohka Kogyo) for the simulation. An electron-beam resist of 1.7 μm thickness is coated on a 1.0-mm-thick silica glass plate. The acceleration voltage of the electron beam is 50 kV, and the development time is 120 s. The residual resist thickness after development is measured for different electron doses. The resist solubility rate R can be expressed as follows using Neureuther's formula(Neureuther et al., 1979):

$$R = R_0 \left(R_1 + \frac{E}{E_0} \right)^\gamma \quad (1)$$

Here, E is the absorbed energy density. The parameters R_0 , R_1 , E_0 , and γ are determined so as to satisfy the above-mentioned experimental results. The absorbed energy density is calculated by electron scatter simulation. The determined parameters R_0 , R_1 , E_0 , and γ are 0.27 nm/s, 1.0, $1.8 \times 10^9 \text{ J/m}^3$, and 4.5, respectively.

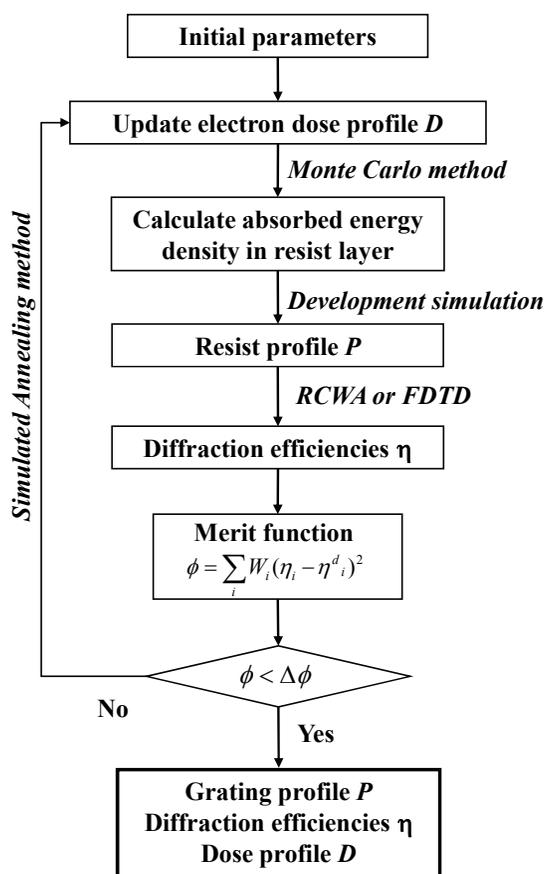


Fig. 1. Optimization flow of DOEs by the electromagnetic grating analysis and the lithography simulation. The optimal design method is called the unified method. The diffraction efficiency is determined from the electric field calculated by the RCWA or the FDTD method. The grating surface profile P and electron dose profile D are optimized simultaneously.

3. Optical design and fabrication results

3.1 Short period diffraction grating

We designed a short period diffraction grating of the electron-beam resist. The grating period is $1.4\ \mu\text{m}$. The refractive indices of the resist and substrate were 1.49 and 1.46, respectively. The light wave of $633\ \text{nm}$ wavelength was normally incident onto the grating, and the light wave is polarized parallel to grating grooves. The resist profile was optimized to obtain the maximum diffraction efficiency for the +1st order diffraction wave. For such a short grating period, the saw-teeth blazed profile does not yield the highest diffraction efficiency.

Figure 2 (a) shows the grating profile designed with the unified method. The calculated diffraction efficiency is 67%. It took about 3 hours to optimize the dose profile by a computer with Compaq Alpha21264 (667 MHz) CPU. The number of iteration was 1000.

We have also designed the grating profile with other designed methods. Figure 2 (b) shows the grating profile optimized only with the RCWA, i.e. the optical optimization process. And the calculated diffraction efficiency is 82%. This diffraction efficiency is higher than that of the suggested optimizing method. However, the grating profile is not easy to be fabricated accurately because of sharp peaks and narrow valleys. Figure 2 (c) is the grating profile designed with the series process, that is, the profile has been optimized under the restriction of the proximity effect as the object profile is Fig. 2 (b). The diffraction efficiency is reduced to 48%, which is about 30% lower than that of Fig. 2 (b). A conventional saw-tooth blazed grating shown as Fig. 2 (d) has the diffraction efficiency of 42%. It is obvious that the grating profile designed with the optimal design method (Fig. 2 (a)) is easy to be fabricated compared with that of Fig. 2 (b). And the diffraction efficiency is superior to those of the saw-tooth blazed grating and the series method.

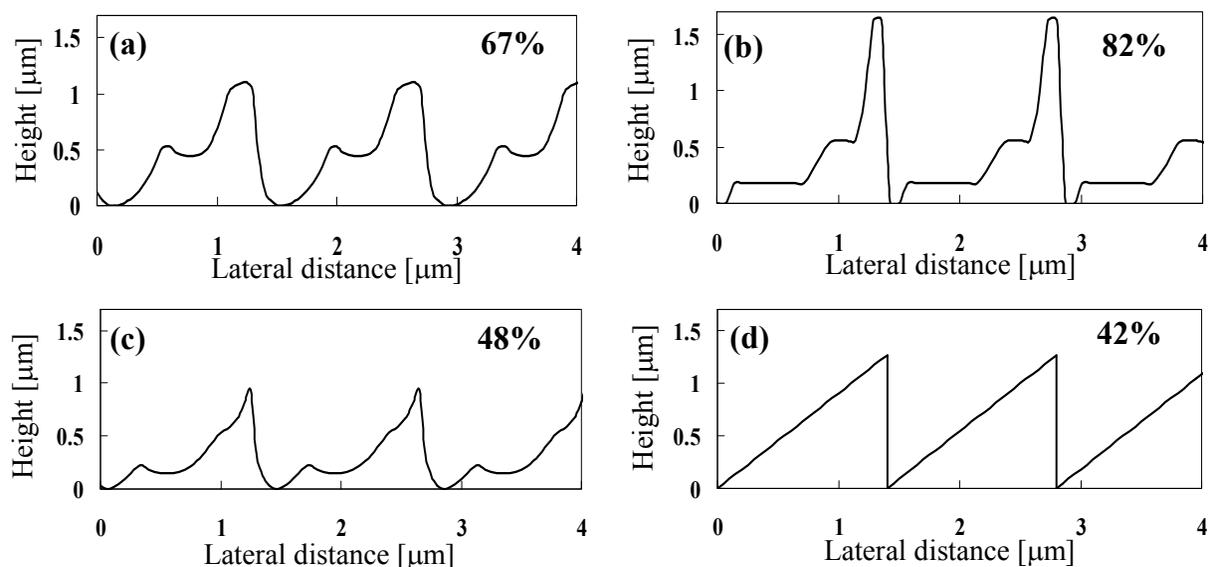


Fig. 2. Grating profiles designed with the different methods; (a) the unified method, (b) the optical optimization process, (c) the series method and (d) a saw-tooth blazed grating, respectively. All of the grating periods are $1.4\ \mu\text{m}$.

Figure 3 shows the grating profiles designed with the unified method for different grating periods, (a) $1.0\ \mu\text{m}$, (b) $1.4\ \mu\text{m}$, (c) $2.6\ \mu\text{m}$ and (d) $6.5\ \mu\text{m}$, respectively. For the long period

grating shown as Fig. 3 (d), the profile becomes the saw-tooth-like blazed profile. On the other hand, for short period gratings, although the optimized grating profile has the round valleys, the diffraction efficiencies are higher than those of the saw-tooth blazed gratings.

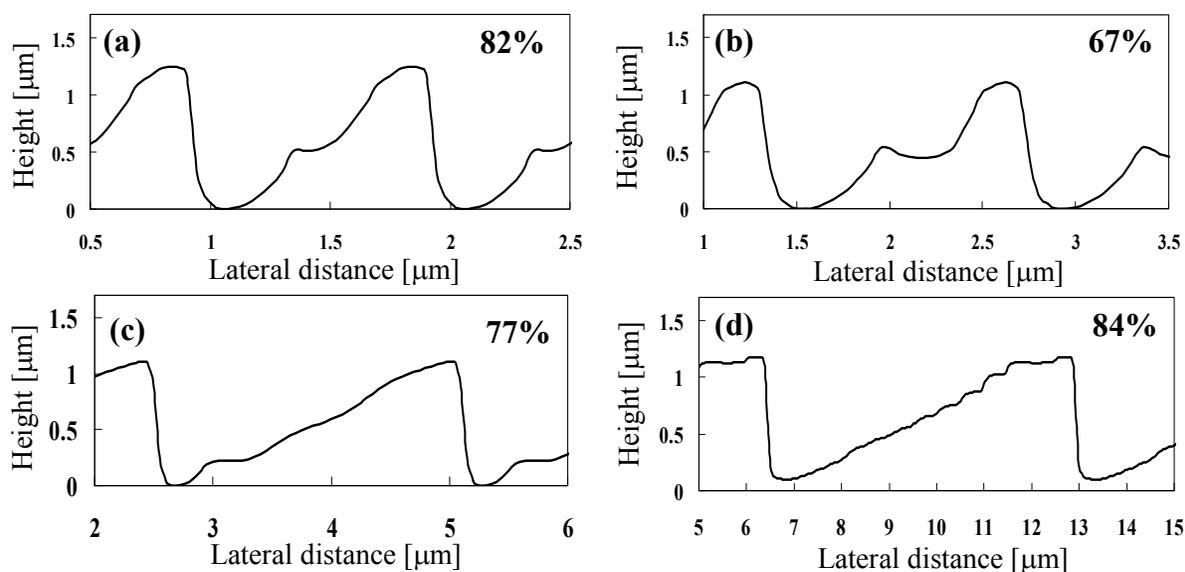


Fig. 3. Grating profiles calculated with the unified method for various grating periods. The grating periods are (a) 1.0 μm , (b) 1.4 μm , (c) 2.6 μm and (d) 6.5 μm , respectively.

The diffraction gratings designed in the previous descriptions have been fabricated with the direct-writing electron-beam lithography. The grating periods were 1.0 μm and 1.4 μm , that is, the grating profiles were Fig. 3 (a) and (b), respectively. We used the electron-beam writer JEOL JBX-5000SI with the acceleration voltage of 50 kV and the beam diameter of 20 nm. The resist thickness was 1.7 μm and the development time was 120 s. The silica glass substrate was 1.0 mm in thickness.

Figure 4 (a) and (d) show the electron-dose profiles calculated with the unified method for the grating periods of 1.0 μm and 1.4 μm , respectively. Though the difference of periods is 0.4 μm , the estimated dose profiles are so different from each other. In the actual fabrication, the electron dosages were according to the calculated dose profiles. The scanning electron microscope (SEM) pictures of the fabricated resist gratings are shown in Fig. 4 (c) and (f). Their surface profiles measured with the atomic force microscopy (AFM) are shown in Fig. 4 (b) and (e), respectively. The grating profiles calculated with the unified method are shown in the figures, too. The grating heights of the AFM profiles are agreed well with those of the calculated profiles. The maximum differences of the profiles are ~ 50 nm. The measured diffraction efficiency was 70% for the 1.0 μm -period grating, and 58% for the 1.4 μm -period grating. These efficiencies are lower by $\sim 10\%$ than the calculated efficiency.

The decrease in diffraction efficiencies is caused by small difference of the grating profiles. In a case of the 1.4 μm -period grating, the diffraction efficiency calculated from the AFM profiles is lower by $\sim 4\%$ than the designed efficiency. The other reason is the stitching error of subfields in the electron-beam writer. The stitching error decreases by a few percents of the diffraction efficiency. To fabricate the grating profile accurately, the resist parameters must be determined more precisely. And the development process also has to be controlled carefully. The stitching error will be reduced by tuning the electron-beam writer.

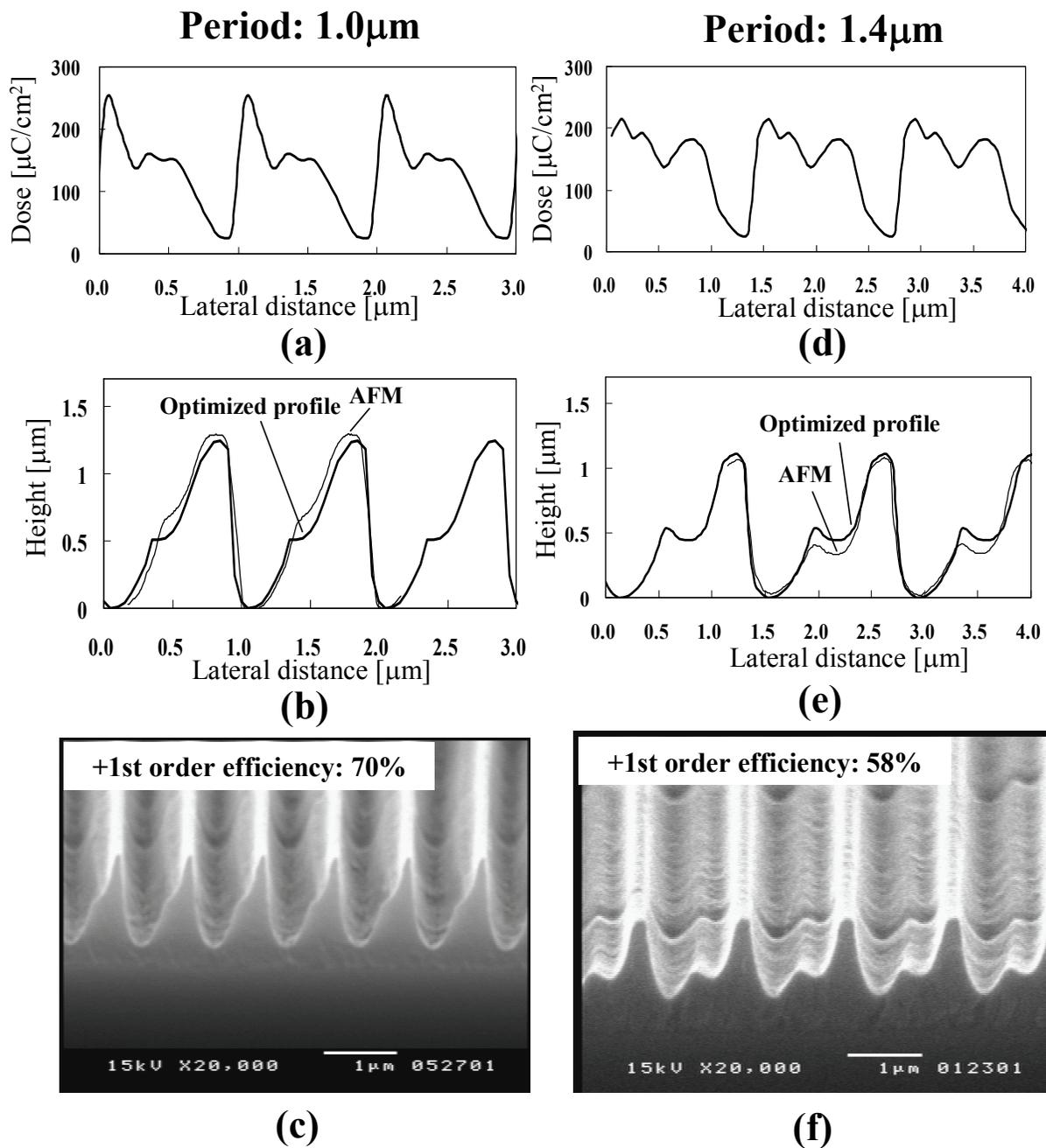


Fig. 4. Fabricated grating profiles. (a) the dose profile calculated with the unified method for the 1.0 μm -period grating. (b) the grating profile measured with AFM and the profile designed with the unified method. (c) the SEM picture of the fabricated grating. (d), (e) and (f) are results for the 1.4 μm -period grating, respectively.

3.2 Diffractive lens

In this section, we designed the diffractive cylindrical lens of an electron-beam resist using the unified method. The diffraction pattern on the focal plane is calculated from the resist profile by the FDTD method. Figure 5 shows the calculation model of the diffractive lens. (x , y) are the coordinates of the field area. To reduce the calculation time and computer

memory, the lens focal plane ($y=y_1$) is not included in the calculation area of the FDTD method. The FDTD method yields the complex amplitude $u(x, y_0)$ immediately above the diffractive lens.

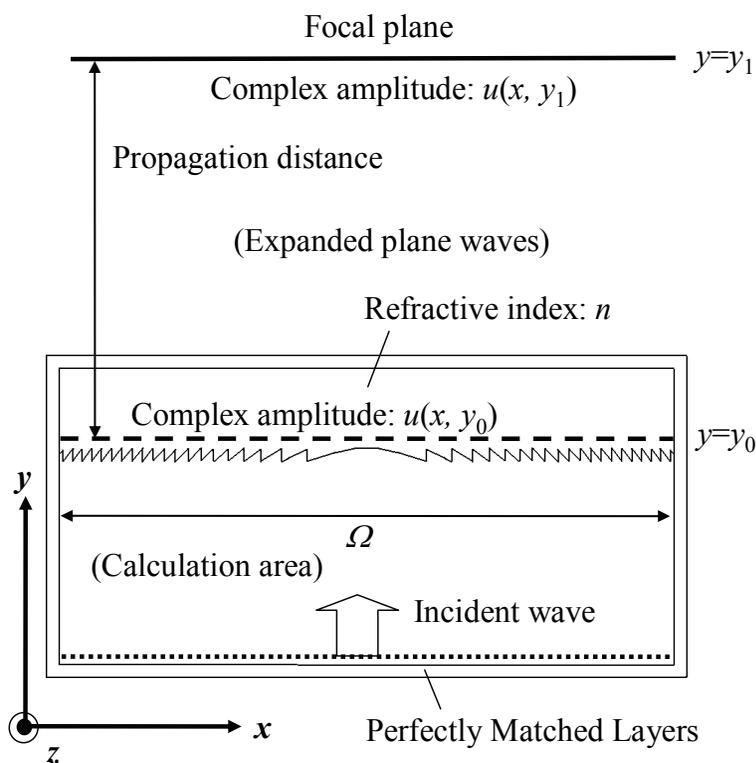


Fig. 5. Estimation of light intensity distribution on focal plane. The incident direction is taken from the substrate to air. The complex amplitude $u(x, y_0)$ of the electromagnetic wave is calculated by the FDTD method. The complex amplitude $u(x, y_1)$ on the focal plane ($y=y_1$) is determined as the integral of Fourier-expanded plane waves.

The electromagnetic field on the focal plane $u(x, y_1)$ is calculated from the amplitude $u(x, y_0)$. $u(x, y_0)$ can be expanded into plane waves by Fourier transform. The complex amplitude of each plane wave $U(k_x)$ is a function of the x component of wave number, k_x , which is expressed as

$$U(k_x) = \int_{-\Omega/2}^{\Omega/2} u(x, y_0) \exp(ik_x x) dx . \quad (2)$$

Ω is the width of the diffractive cylindrical lens. The complex amplitude on the focal plane $u(x, y_1)$ becomes

$$u(x, y_1) = \frac{1}{2\pi} \int U(k_x) \exp[ik_y(y_1 - y_0)] \exp(-ik_x x) dk_x . \quad (3)$$

k_y is the y component of wave number expressed as

$$k_y = \sqrt{(2\pi n / \lambda)^2 - k_x^2} , \quad (4)$$

where λ is the wavelength of light in a vacuum and n is the refractive index of light-propagating media. The intensity distribution $I(x)$ on the focal plane is the absolute square of $u(x, y_1)$.

We defined the merit function as an integral of the mean square of the difference:

$$\phi = \int [I(x) - I_d(x)]^2 dx, \quad (5)$$

where $I_d(x)$ is the desired intensity distribution. We set the diffraction limit of the cylindrical lens as the desired intensity profile $I_d(x)$, which is expressed as

$$I_d(x) = \text{sinc}^2\left(\frac{\Omega n}{f\lambda} \pi x\right). \quad (6)$$

Here, $\text{sinc}(x) = \sin(x)/x$. The diffraction-limit width w is given by

$$w = 2 \frac{f\lambda}{\Omega}, \quad (7)$$

where f is the focal length. The focus efficiency is defined as the ratio of the energy contained in the diffraction-limit width w to the energy incident to the cylindrical lens.

If the merit function ϕ is greater than a certain tolerance value, the electron dose profile D is modified. It is described that the simulated annealing algorithm can be used for the modification of electron dose. The above-mentioned calculations are iterated until the merit function ϕ is less than the admissible value or until it converges well. The outputs of the optimal design are the electron-dose profile D , resist surface profile P and intensity distribution $I(x)$ on the focal plane.

The designed diffractive cylindrical lens is 50 μm in width and the focal length is 25 μm for the 650-nm-wavelength light. The diffraction-limit width w becomes 0.65 μm . Since the designed lens has an F -number of 0.5, the middle zone has a parabolic surface profile of 11.4 μm width. The second zones next to the middle are 2.43 μm wide, and both end zones are 0.93 μm wide. The total number of grating periods and the parabolic surface profile is 31. A polarized light wave is normally incident to the diffractive lens from the substrate. The electric field of the incident light is normal to the x - y plane. The refractive indices of the substrate and grating material are 1.46 and 1.49, respectively.

The grid size of FDTD calculation is 50 nm square. The calculation area consists of 1199 \times 109 cells and is surrounded by perfectly matched layers. The electron dose is modulated by 9-58 levels, which depends on the grating period. The calculation time for one process from giving the dose profile to evaluating the diffraction efficiency is 11 min. After 120 iterations, the diffraction efficiency practically converges. The total calculation time for the optimization is about 22 h using a computer with an AMD Athlon 1.2 GHz CPU.

Figure 6 shows the results of the optimal design. The dose and calculated resist profiles are shown in (a) and (b), respectively. The dose profile is complex and the calculated profile is very different from the conventional wrapped parabolic surface profile. Figure 6 (c) shows the calculated intensity distribution on the focal plane. The focus efficiency is 49%. Figure 7 shows the conventional wrapped parabolic surface grating and its intensity distribution. Its focus efficiency is 37%. The efficiency of the optimized diffractive lens is significantly higher

than that of the conventional diffractive lens. The focus efficiency of the optical optimization without the lithography simulation is 53%.

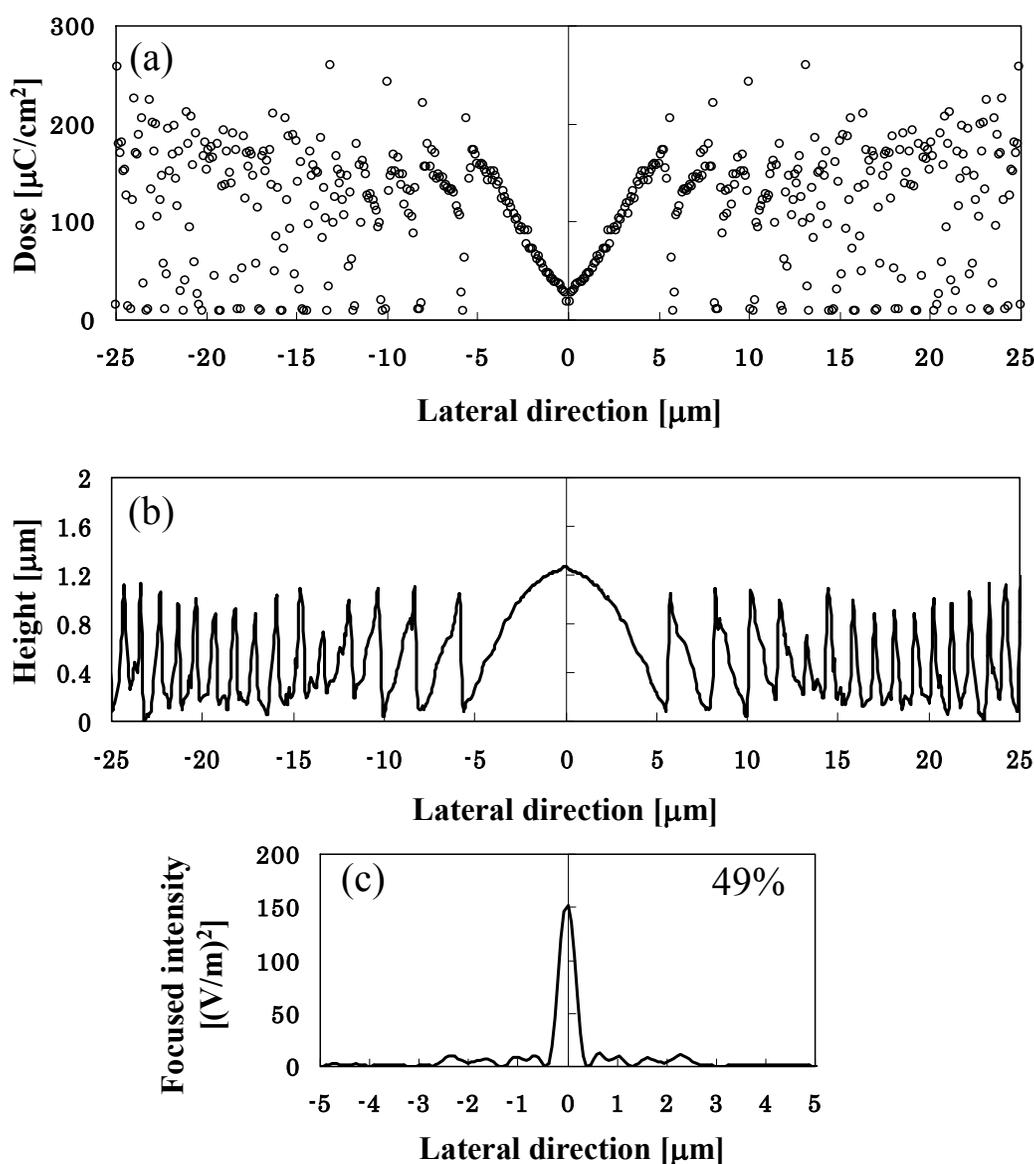


Fig. 6. Diffractive cylindrical lens designed by the unified method: (a) estimated dose profile, (b) calculated resist profile, and (c) light intensity profile on focal plane.

4. Conclusions

We suggested the unified design method of grating profiles with the electromagnetic grating analysis and the electron-beam lithography simulator. The unified method gives us the optimum grating profile and the electron dose profile under the restriction of the proximity effect of the electron scattering. This method is useful especially for short-period gratings. The conventional design method based on only the electromagnetic grating analysis yields the theoretical highest diffraction efficiency. However, the calculated grating profiles may be too complex to be fabricated, so that such a high efficiency will not realized.

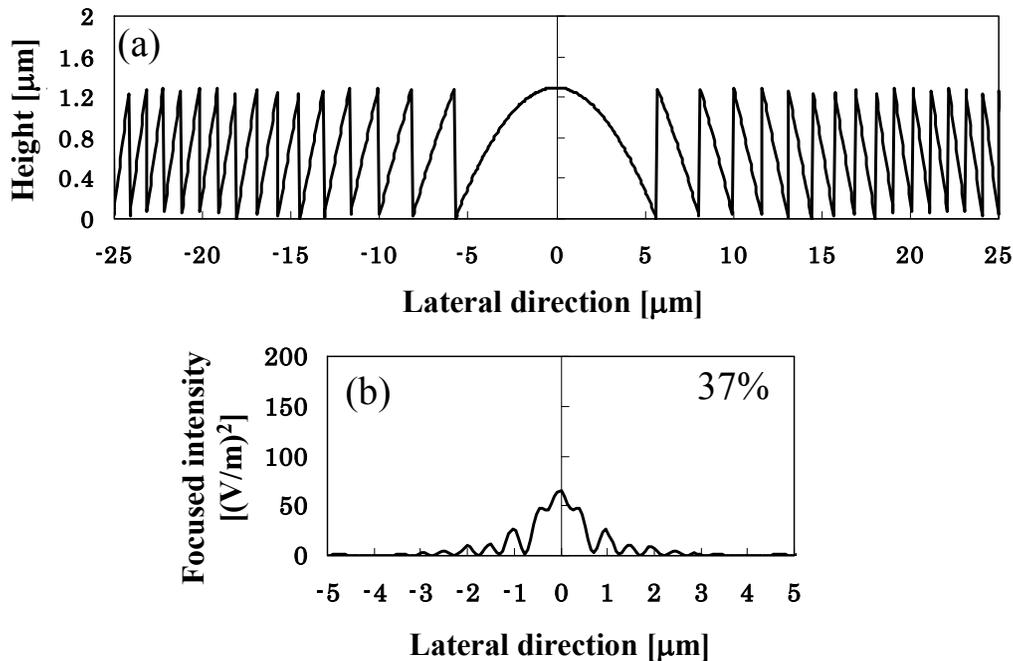


Fig. 7. Conventional wrapped parabolic diffractive lens: (a) cross-sectional profile, and (b) calculated light-intensity profile on focal plane.

On the other hand, the unified method gives us the fabricatable grating profile and the highest diffraction efficiency under the restriction of the proximity effect.

Moreover, the unified method enables to calculate nonperiodic DOEs as diffractive lenses using the FDTD method. The focus efficiency of diffractive lens with small F -number is significantly higher than that of the conventional diffractive lens with the saw-tooth blazed grating profiles. However, a long calculation time is required. Parallel computation is suitable for wide diffractive lenses, because both the FDTD method and the lithography simulation are appropriate for parallel computation.

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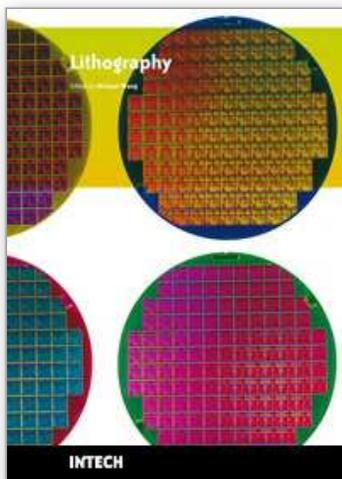
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