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Dielectric binary blazed gratings

H. Haidner, J. T. Sheridan, and N. Streibl

Artificial index gratings, which are composed of binary microstructures of sizes less than the incident wavelength, are analyzed as functions of the filling factor or duty cycle of the microstructures. Different models for calculating the optimum duty cycles to produce high blazed diffraction efficiency are compared. Blazed binary grating designs in a material with a refractive index $n = 2$ show theoretical diffraction efficiencies as high as $\eta = 80\%$. In the semiconductor material silicon, which has a refractive index $n = 3.4$, theoretical diffraction efficiencies as high as $\eta = 70\%$ are predicted.

Conventional blazed gratings consist of grooves with a sawtooth profile. Recently¹⁻⁴ it was proposed that instead subwavelength microstructures of binary profile with a variable duty cycle (or filling factor) be used. Since each microstructure is much smaller than the wavelength, averaging, analogous to the index averaging in a dielectric zero order grating, takes place inside each microstructure. By modulating, for example, the duty cycle, as is shown in Fig. 1, the microstructure can be made to behave analogously to a distributed index material with a gradient refractive index. By periodic repetition of M such microstructures with modulated duty cycles t_m , where $m = 1, \dots, M$, a blazed grating with high diffraction efficiency can be constructed of binary features.

In this Technical Note it is assumed that the change in the duty cycle between neighboring microstructures is small and that in this case each microstructure acts as though it is one period of a zero order grating, the duty cycle acting as a perturbing variable. In this case when the duty cycle changes adiabatically, or slowly, it is assumed sufficient to know the phase delay caused by a homogeneous zero order grating with a duty cycle $t_m = d_{3,m}/d_2$ that defines the phase delay at points along the entire superlattice period d_1 . The theory of form birefringence,⁵ also referred to as the small-period approximation (SPA), leads to an average dielectric constant $\epsilon_{av,m}$ for this grating of

$$\epsilon_{av,m} = n_1^2(1 - t_m) + n_2^2 t_m. \quad (1)$$

This translates into an expected phase delay $\varphi_{d,m}$ (Refs. 1-3) for TE-polarized light $\varphi_{d,m}$ of

$$\varphi_{d,m} = (2\pi h/\lambda)[n_1^2(1 - t_m) + n_2^2 t_m]^{1/2} - 2\pi h n_1/\lambda. \quad (2)$$

This approximation holds for very fine gratings, $d_2 \ll \lambda$. However, structures with larger periods are easier to fabricate and can be analyzed by rigorous diffraction theory, e.g., the differential method (DM).⁶ When the SPA is valid, one can invert Eq. (2) to obtain an appropriate duty cycle t_m for a fixed phase $\varphi_{d,m}$. If the SPA is not valid, the phase $\varphi_{d,m}$ as a function of the duty cycle t_m can be calculated by using the DM, and then the computed function can be inverted. In each methodology a required phase is assigned to each subsection along the large period d_1 . This localized phase delay must then be translated into a corresponding duty cycle. With our methods the phase from a zero order grating calculated by using SPA or DM is plotted as a function of the zero-order-grating duty cycle. We then placed the resulting large-period, cross-sectional Fourier permittivity expansion designed in this way into the DM to calculate the corresponding diffraction efficiency of the artificial index grating (AIG).

Recently a third method,⁴ called here the F method, for calculating the duty cycle of the AIG was proposed. This model does not deal with the idea of an average refractive index derived by considering zero order gratings. Instead, by comparing the Fourier series of the cross-sectional permittivity of a continuous graded-index grating with that of an AIG, it is deduced that an appropriate choice of the duty cycles is given by the linear equation

$$t_m = m/(M + 1). \quad (3)$$

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Fig. 1. AIG with period d_1 made up of M microstructures, each of size d_2 . The grating depth is h . Each microstructure is different because of the variation in the filled part of the microstructure $d_{3,m}$.

In Fig. 2 the duty cycle as a function of the phase, the inverted function, is presented as predicted by the SPA, DM, and F methods. The refractive indices are $n_1 = 1$ and $n_2 = 2$. The height of the microstructure is $h = 1 \mu\text{m}$, the wavelength $\lambda = 1 \mu\text{m}$, and the microstructure pitch $d_2 = 0.4 \mu\text{m}$. The F function is a straight line because of Eq. (3). The SPA function is below the F function, as is the DM function. The DM function takes the size of the zero order grating d_2 and higher-order evanescent waves into account and is therefore more physically accurate than the SPA function. Now the three methods for choosing the duty cycles of a microstructure are used to design optimum AIG's. In Fig. 3 the diffraction efficiencies of the +1.0 order of the three proposed AIG's are presented as functions of the depth. The gratings are composed of $M = 10$ microstructures of the kind described in Fig. 2 and therefore have a period $d_1 = 4 \mu\text{m}$; the other parameters are the same as in Fig. 2. The SPA, DM, and F functions of Fig. 2 are used to determine appropriate duty cycles t_m . Then the diffraction efficiencies of the three gratings are calculated with the DM, $N = 41$ diffracted orders being included in the calculation. The AIG that results from using the DM prediction shows most diffraction efficiency in the +1.0 order, $\eta \approx 81\%$. The efficiency of the grating using the SPA prediction has a maximum diffraction efficiency of $\sim 76\%$, and the grating resulting from the F prediction has the lowest maxi-

Fig. 2. Duty cycle as a function of phase: F, SPA, and DM predictions are presented for a microstructure with $d_2 = 0.4 \mu\text{m}$, $h = 1 \mu\text{m}$, $n_1 = 1$, $n_2 = 2$, $\lambda = 1 \mu\text{m}$, and normal incidence.

Fig. 3. Diffraction efficiency of the +1.0 order as a function of depth. The three gratings consist of $M = 10$ microstructures. The duty cycles t_m of the microstructures were chosen with the help of the SPA, DM, and F functions in Fig. 2. The physical parameters of the microstructures are the same as those in Fig. 2.

mum diffraction efficiency, $\sim 70\%$. It should also be noted that this grating has its maximum diffraction efficiency at a greater depth, $h_F = 1.4 \mu\text{m}$, whereas $h_{SPA} = 1.1 \mu\text{m}$. Depth is an important issue since the difficulty in fabrication increases with the aspect ratio and therefore with the depth of the microstructure.

In Fig. 4 the diffraction efficiencies of the +1.0 diffracted order of a grating, made in a semiconductor material for IR operation, as functions of the depth h are presented. The grating has a period $d_1 = 30 \mu\text{m}$, refractive indices $n_1 = 1$ and $n_2 = 3.4$, and $M = 10$ microstructures of size $d_2 = 3 \mu\text{m}$. The choices of the duty cycles were made with the SPA prediction, the DM prediction, and the F prediction. The normally incident plane wave is TE polarized and has a wavelength λ of $10.6 \mu\text{m}$. The diffraction efficiencies of the gratings were calculated, after the duty cycles of the microstructures were chosen, by using the DM. $N = 61$ diffracted orders were included in the calculation. The grating designed with the DM shows the most diffraction efficiency, $\eta \approx 70\%$, at a depth $h_{DM} = 4.5 \mu\text{m}$. Again the grating based on the SPA prediction has higher efficiency in the +1.0 order, $\eta \approx 57\%$, than the grating based on the F prediction with $\eta \approx 53\%$. Also the F prediction shows the maximum of the diffraction efficiency of the +1.0 order at a greater

Fig. 4. Diffraction efficiency of +1.0 diffraction order as a function of depth: $d_1 = 30 \mu\text{m}$, $d_2 = 3 \mu\text{m}$, $n_1 = 1$, $n_2 = 3.4$, $\lambda = 10.6 \mu\text{m}$, and normal incidence. Three gratings with $M = 10$ microstructures, designed using the F, DM, and SPA methods to choose the optimum duty cycles, are compared.

depth, $h_F = 6 \mu\text{m}$, than the SPA prediction with $h_{\text{SPA}} = 4 \mu\text{m}$.

Numerical calculations have also been carried out in a great number of other cases. In this investigation physical practical values of the superlattice period d_1 , the number of microstructures M , the refractive index n_2 , and the incident wavelength have been examined. In all cases it was found that choosing the duty cycles of an AIG by using the idea of the average index, based on the model of a zero order grating, produces a stronger blazed effect than matching the Fourier components. The reason for this appears to stem from the results in Fig. 2. When one is dealing with a zero order grating, the SPA gives a nonlinear response to duty-cycle change, which more closely resembles the corresponding DM response than the F method. In the SPA method one starts with a better birefringent effective index approximation and therefore can achieve higher blazed efficiency.

It should be pointed out that when nonlinear optimization techniques are used, such as the steepest ascent/descent method or simulated annealing, higher efficiencies than those predicted with any of

the methods above should be achievable. We believe, however, that the SPA technique offers a natural best starting point for any optimization procedure.

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