Diffractive optics based on modulated subwavelength-domain V-ridge gratings

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Abstract
We study the properties of reflection-type V-ridge gratings in the subwavelength domain and describe a method to realize diffractive optical elements by using such gratings as signal carriers. In particular, we utilize a coding scheme based on position modulation of a high-frequency V-ridge carrier grating. We design and demonstrate beam splitting elements using this coding scheme, electron-beam lithography, anisotropic wet etching of silicon, hot embossing of polymer, and metal deposition. These elements have the outstanding property of operating over a large spectral range from 406 to 520 nm. The measured diffraction patterns show excellent agreement with theoretical results given by rigorous diffraction theory.

Keywords: diffraction, gratings, subwavelength optics, beam splitting, lithography, wet etching

(Some figures may appear in colour only in the online journal)

1. Introduction

Realization of diffractive elements by modulation of high-frequency carrier gratings has its origin in off-axis optical holography [1]. An alternative approach to generate diffractive elements is the computational scheme introduced by Lohmann [2]. By early 1990s such synthetic methods had reached a level that allowed the design of high-quality elements with optimized diffraction efficiency using iterative techniques [3]. In this period the technological development of lithographic fabrication techniques allowed the encoding of these design in different types of wavelength-scale carrier structures; see [4] for a review of many of these coding methods and [5, 6] for examples of recent advances in fabrication technology.

One of the coding methods employs modulated high-frequency carrier gratings in the spirit of optical holography [7–9]. In these studies binary gratings were used as carriers, providing high transmission-mode efficiency when the carrier period is close to the wavelength and the angle of incidence is close to the Bragg angle. The binary coding scheme can also be used in the reflection mode, in which case the high efficiency can be maintained over a much wider range of incident angles (note that the analysis of reflection gratings in [8] was restricted to perfectly conducting case, but the same general conclusion holds also for gratings with finite conductivity).

We propose a new method to realize high-carrier-frequency diffractive elements as an alternative to binary resonance-domain structures. In terms of optical performance, these two are comparable. However, the wet etching technique [10] employed here facilitates more precise control of groove shape and easier replicability of the structures. In the recent advances, the wet etching of silicon has triggered a new era in the production of photovoltaic devices [11–13]. In the past such gratings have been proposed for spectroscopy [14–16], infrared beam splitting [17, 18], reflection suppression [19, 20] and optical interconnection [21]. Here we apply inverted V-groove gratings, which we call V-ridge gratings, as carriers of reflection-type diffractive elements, realizing the optical function by lateral position modulation of subwavelength-structured V-ridges. We employ modulation profiles designed to split the incident beam into output beams of equal efficiency since such elements are easy to characterize both theoretically and experimentally. We apply rigorous diffraction theory to study conditions under which...
good signal quality can be achieved. An experimental demonstration is provided by wet etching the modulated grating structure in Si, subsequently replicating it in polymer, and finally coating the replicated structure with a thin metal layer.

2. Properties of the reflective carrier grating

Let us begin by considering figure 1, which illustrates both the structure of the V-ridge carrier grating and the principle of ridge-position modulation. The carrier grating of period \( d \) has symmetric V-ridges with apex half-angle \( \alpha = 35.26^\circ \) and width \( w \), separated by flat surface sections of width \( d - w \). When the carrier is modulated, the ridge width is kept constant but the tip positions \( s_n \) are chosen according to the coding scheme to be employed. Because of fabrication constraints, the modulation should be sufficiently slow to ensure that the widths \( d - w \) of all flat regions are at least \( \sim 50 \) nm.

Since position modulation has no effect in the phase of the zeroth generalized order of the structure, we concentrate on the (minus) first order \( m = -1 \) of the carrier grating. To achieve high efficiency in this order we choose the angle of incidence \( \theta \) and the carrier period \( d \) in such a way that the only propagating reflected orders are \( m = -1 \) and \( m = 0 \). We then optimize \( w \) to obtain maximum efficiency \( \eta_{-1} \) in order \( m = -1 \). This is achieved by a simple scan of \( w \), using the Fourier modal method (FMM) with the S-matrix propagation algorithm [22] to evaluate the diffraction efficiencies. As illustrated in figure 2, the wedge region is divided into \( J \) layers thin enough to model the continuous facets with sufficient accuracy. We assume illumination by a TM polarized (magnetic field in \( y \) direction) monochromatic plane wave and, in the design, assume that the Bragg condition holds (Littrow mounting) for the design wavelength \( \lambda_0 \):

\[
\sin \theta = \frac{\lambda_0}{2d}
\]  

Typically we chose \( J = 35 \) and included \( \sim 50 \) Floquet–Bloch modes in the calculation of carrier-grating efficiencies.

In what follows, we consider a design wavelength \( \lambda_0 = 457 \) nm and assume that the metal is (bulk) aluminium with complex refractive index \( 0.6402 + i5.5505 \). We have some freedom to choose the carrier period \( d \) or the angle of incidence \( \theta \). The results for several choices of these parameters are shown in figure 3. In figure 3 we plot the results for three different values of the angle of incidence, \( \theta = 30^\circ, 42^\circ, \) and \( 60^\circ \), while keeping the carrier period at a fixed value \( d = 340 \) nm. Remarkably, for all values of \( \theta \), the optimum solution with \( \eta_{-1} \approx 87\% \) is achieved with a ridge width \( w \approx 220 \) nm corresponding to a fill factor \( w/d \approx 0.64 \). For comparison, the reflectance of a flat air-aluminium interface at these angles of incidence varies in the range 86\%–91\%. In fact, the zeroth-order efficiency virtually vanishes at the optimum value of \( \eta_{-1} \), which means that the latter is limited by absorption. In view of figure 3(b), the value of \( d \) is not critical either. We obtain essentially the same optimum \( \eta_{-1} \) at the same value of \( w \) as above for all carrier periods \( d \) considered.

The dashed lines in figure 3 show results for TE polarized light with \( \theta = 42^\circ \) in (a) and \( d = 340 \) nm in (b). We see that the efficiency is limited to \( \sim 50\% \) if we leave some room for modulation. The reason for these low efficiencies is that TE polarized light cannot penetrate deep inside the grooves of metallic subwavelength-period gratings, which prevents sufficient phase modulation for high diffraction efficiency to be
achieved. The situation is analogous to that encountered in binary subwavelength-period metallic gratings (see, e.g., [23]). Note that for this wavelength and at this period, aluminium is a good plasmonic material but the optimized period is too small to see any plasmon resonance. But of course making use of elevated Fermi level of graphene such metallic properties could be altered. Recently, the graphene supported metamaterials have shown new directions in the tunability of the metallic properties [24–26].

3. Coding of high-frequency V-ridge structures

Referring to figure 1, the modulation of the carrier is determined by the shifts $s_n$ of the ridge tips with respect to their undisturbed positions $x_n = (n - 1/2)d$ in the carrier grating. These shifts are determined by the phase-only modulation function $\phi(x)$ to be encoded in the element using the detour-phase principle [2]. Denoting the sampled values of $\phi(x)$ at $x_n$ by $\phi_n$ we have

$$S_n = \frac{\phi_n \cdot d}{2\pi}. \quad (2)$$

The modulation function $\phi(x)$ can be, e.g., that of a lens, a beam shaping element, or any numerically constructed phase function designed by the methods of diffractive optics [27] to convert an incident plane wave into a predefined angular spectrum of plane waves within some signal window $W$. Among the available design techniques are various parametric optimization methods and the iterative Fourier-transform algorithm (IFTA) [3, 27], which we use to design the elements.

The main requirement concerning the phase function $\phi(x)$ in the present coding scheme is that it varies slowly compared to the carrier period in the sense that

$$|s_n - s_{n+1}| \ll d \quad (3)$$

for all $n$. Under this condition adjacent ridges do not overlap, except perhaps at points where the phase of $\phi(x)$ changes abruptly. Such points occur inevitably if $\phi(x)$ is wrapped in the $[0, 2\pi]$ interval, but in many designs one also encounters phase jumps other than $2\pi$ radians, which cannot be unwrapped. Whether $\phi(x)$ is wrapped or not, we assume it to vary slowly enough to ensure that these isolated phase jump points are sufficiently far apart to cause only local disturbances in the coded profile.

In our examples we consider periodic elements that satisfy the condition $\phi(x + D) = \phi(x)$, where the so-called superperiod $D$ is taken to be a multiple of the carrier period $d$, i.e., $D = Nd$ as illustrated in figure 1. Then the carrier order $m = -1$ is split into a discrete angular spectrum of plane waves, which correspond to the diffraction orders of an on-axis element with phase function $\phi(x)$. Note that although the superperiod is taken into account the plasmon will not appear because the ridges are now unevenly spaced. In order to satisfy the condition (3), the effective spread of the angular spectrum containing the intended signal window $W$ must be small compared with the diffraction angle of the carrier order $m = -1$, i.e., the diffraction geometry should be parbasal. We proceed to investigate this point more quantitatively using numerical examples.

4. Numerical examples

In the following examples we consider beam splitter gratings that divide the incident plane wave into an array of a total number of $Q$ plane waves with equal efficiencies. We refer to the index of the orders of the modulation grating with period $D = Nd$ by symbol $q$ and from now on $\eta_q$ denotes the diffraction efficiency of order $q$. Hence the total efficiency within the set $W$ of signal orders is

$$\eta = \sum_{q \in W} \eta_q \quad (4)$$

and the array uniformity error is defined as

$$E = \frac{\max \eta_q - \min \eta_q}{\max \eta_q + \min \eta_q} \quad (5)$$

Figure 3. Efficiency of carrier order $m = -1$ for (a) different incident angles and (b) different carrier periods when the wedge width $w$ is varied. The solid lines refer to TM polarized light and the dashed line to TE polarized light.
with \( q \in W \). Note that, after modulation of the carrier grating, order \( q \) in the axial design corresponds to order \( q - N \) of the superperiodic grating.

We employ the FMM to investigate the effect of \( N \) in the performance of ridge-position modulated gratings. In all examples considered below we take \( \lambda = 457 \) nm, \( \theta = 42^\circ \), and \( d = 340 \) nm. In order to obtain good convergence, the number of diffraction orders included in the FMM analysis was in all cases taken to be at least \( \sim 30N \). The bulk refractive index of Al was used to model the metal substrate, assumed semi-infinite as in figure 1.

Let us begin with a triplicator \( (Q = 3) \), for which the optimum continuous profile \( \phi(x) \) is known analytically \([28]\) and produces a total efficiency \( \eta = 0.92556 \) into orders \( q = -1, 0, +1 \) that make up \( W \). Figure 4 illustrates the discrete \( N = 16 \) bit design of \( \phi(x) \) and the resulting on-axis diffraction pattern calculated within the thin-element approximation. The efficiency is \( \eta \approx 0.926 \) and the array uniformity is virtually perfect.

Figure 5(a) illustrates the result on FMM analysis of a modulated triplicator with \( N = 16 \) bits. On comparing this result with figure 4(b) we see that the array is somewhat distorted and there is some residual light in the central region of the pattern, which corresponds to the location of order \( m = 0 \) of the carrier grating (the zeroth generalized order of the modulated grating). The uniformity error is due to the fact that, with \( N = 16 \), the geometry is not yet sufficiently paraxial to fully justify the condition (3). In view of figures 5(c) and (d), increasing \( N \) improves the uniformity as expected. Table 1 illustrates the results of the FMM analysis more quantitatively. The diffraction efficiencies of the encoded elements are close to the expected value, which is the efficiency of the axial design (92.6\%) multiplied by the efficiency (87\%) of the carrier grating, i.e., \( \sim 80.6\% \).

An analysis similar to that presented above for triplicators has also been performed for array illuminators that generate five beam in orders \( q = -2, \ldots, +2 \) and eight beams in orders \( q = -3, \ldots, +4 \). In the former case the efficiency given by IFTA is \( \eta \approx 0.92 \), and in the latter case \( \eta \approx 0.96 \). In both cases the array uniformity is again virtually perfect. While the profile \( \phi(x) \) of the triplicator was limited within the \([0, 2\pi]\) interval, this is no longer the case for the \( Q = 5 \) and \( Q = 8 \) designs. In the \( Q = 5 \) case we unwrapped the one \( 2\pi \) phase jumps and encoded the resulting profile. In the \( Q = 8 \) case we first unwrapped \( \phi(x) \), then shifted its minimum to \(-\pi\), and finally wrapped the profile again. This procedure minimizes the number \( 2\pi \) phase jumps to 2. An unwrapped profile could be used as well, but the (continuous) phase function \( \phi(x) \) of the \( Q = 8 \) design contains one phase jump of \( \pi \) radians, which cannot be unwrapped.

The quantitative results for the \( Q = 5 \) and \( Q = 8 \) designs are presented in tables 2 and 3, respectively. As expected, if we increase \( Q \) while keeping \( N \) constant, the uniformity error increases. However, the uniformity again improves when \( N \) is increased. In the case of the \( Q = 8 \) design, rewrapping \( \phi(x) \) improved the uniformity error somewhat, which was not initially expected.

5. Effects of varying the wavelength and angle of incidence

We proceed to consider the case of input plane waves arriving at different angles and having different wavelengths, concentrating here on the triplicator case since the other designs behave analogously. The effects of varying the wavelength \( \lambda \) are shown in figure 6(a), where the spectral sampling interval is 0.6 nm and the wavelength dependence of the refractive index of Al is taken into account. The efficiencies of signal orders \( q \approx 1 \) (blue), \( q = 0 \) (green), and \( q = -1 \) (red) vary relatively little over the spectral region spanning from 400 to 500 nm. Note that order \( q = -1 \) vanishes because of a Rayleigh anomaly at \( \lambda = 535 \) nm. At this stage the design principle breaks down and the efficiency of the zeroth carrier order increases rapidly. Figure 6(b) illustrates the angular tolerances of the triplicator with \( N = 16 \). The signal orders...
show only a weak dependence on the incident angles in the range $36° - 64°$, which in turn implies a high angular tolerance of the element. This tolerance becomes even better with larger $N$ since the angular spread of $W$ reduces.

### 6. Fabrication

A process flow for fabricating the V-ridges into cyclo-olefin-copolymer (COC) is presented in figure 7(a). We fabricated and tested a triplicator with $N = 16$. In the first step of the process, 250 nm of the thermal oxide layer was grown on the standard silicon (100) wafer. Then a 200 nm thick electron beam resist layer (ZEP 7000) was spun on the substrate. Next step was followed by electron beam exposure of the grooves using Vistec EBPG 5000 + ES at 100 keV. The exposed resist layer was developed in EEP, followed by reactive ion etching of the thermal oxide layer in step (3). This layer was used as a mask in silicon wet etching using 30% KOH at 70 °C. This resulted in grooves with $\alpha = 35.26°$ defined by the wet etching characteristics of the (100) silicon wafer in step (4). The groove widths were defined by the e-beam exposure. Finally, in step (5) the thermal oxide was removed in buffered oxide etch.

The silicon master was utilized in hot-embossing of COC using Obducat Eitre 3 nanoimprinter. As a final step, the resulting triangular ridges were coated with $h = 70$ nm sputtered aluminum layer, resulting in a type of profile illustrated in figure 8.

### 7. Experimental results

Next we discuss the experimental setup shown in figure 9 and the corresponding measurements. The setup has two parts,
one for aligning the tilt orientation of the beam using mirrors M1 and M2 and the other is for grating measurements. Here we concentrate on the first part because this allowed us to separate the input laser beam from the array of reflected beams to permit all measurements; the other part will be discussed in the following section. A diode pumped solid state laser operating at central wavelength $\lambda = 457$ nm having beam width of 3 mm with a maximum output power of 29 mW is used in the experiments. The horizontally polarized light is now incident onto the grating having size $4 \times 5$ mm upon successive reflection from the mirrors.

We measured the fabricated triplicator at $\lambda = 457$ nm at an angle of incidence $\theta = 38^\circ$, while the Bragg angle is $42^\circ$. The experimental results were compared with FMM simulations, where the finite thickness of the metal layer was taken into account. In modeling the metal, we used the refractive-index data for thin films of sputtered Al [29]. The refractive index of the COC polymer was taken to be 1.53. By scanning the diffraction pattern with a detector we determined the efficiencies of orders $q - N = -17$ (red), $q - N = -16$ (green), $q - N = -15$ (blue), and $q - N = 0$ (black) as a function of (a) wavelength and (b) angle of incidence.

![Figure 6](image_url) Simulation results for the pulse-position-modulated triplicator with $N = 16$. Efficiencies of orders $q - N = -17$ (red), $q - N = -16$ (green), $q - N = -15$ (blue), and $q - N = 0$ (black) as a function of (a) wavelength and (b) angle of incidence.

| Signal orders | $N$ | $\eta_2$ | $\eta_1$ | $\eta_0$ | $\eta_{-1}$ | $\eta_{-2}$ | $\eta$ | $E$ (%) | DO | $D$ ($\mu$m) |
|---------------|-----|---------|---------|---------|-----------|-----------|-------|--------|----|---------|
| 32            | 0.148 | 0.167 | 0.158 | 0.141 | 0.165 | 0.779 | 8.4 | 2500 | 10.88 |
| 64            | 0.153 | 0.163 | 0.158 | 0.151 | 0.161 | 0.786 | 3.8 | 3500 | 21.76 |
| 128           | 0.149 | 0.153 | 0.150 | 0.147 | 0.152 | 0.751 | 2.0 | 4000 | 43.52 |

Table 2. The same as table 1 but for 5-beam designs.

| Signal orders | $N$ | $\eta_4$ | $\eta_3$ | $\eta_2$ | $\eta_1$ | $\eta_0$ | $\eta_{-1}$ | $\eta_{-2}$ | $\eta_{-3}$ | $\eta$ | $E$ (%) |
|---------------|-----|---------|---------|---------|---------|---------|-----------|-----------|-----------|-------|--------|
| 32            | 0.103 | 0.109 | 0.090 | 0.108 | 0.082 | 0.109 | 0.098 | 0.082 | 0.782 | 14 |
| 64            | 0.101 | 0.105 | 0.102 | 0.103 | 0.092 | 0.106 | 0.101 | 0.095 | 0.806 | 6.8 |
| 128           | 0.094 | 0.096 | 0.100 | 0.093 | 0.096 | 0.100 | 0.100 | 0.097 | 0.776 | 3.6 |

Table 3. The same as table 1 but for 8-beam designs. The values of DO and $D$ (not shown) are the same as in table 2.
agreement. Note that the design principle fails at \( \lambda = 633 \text{ nm} \) since all signal orders become evanescent. However, the measured value of zeroth-order efficiency is in good agreement with the theoretical result.

8. Conclusions

We introduced a position coding method of reflection-type diffractive elements, making use of high-frequency V-ridge carrier gratings. The position modulation scheme was demonstrated by fabricating a triplicator for visible light using wet etching of silicon, nanoimprint lithography and metal deposition. Electron beam lithography is only required for the master fabrication where positions of the grooves are modulated with high precision. This fabrication scheme allows large-scale production of diffractive structures. The fabricated element was shown to possess a remarkable spectral and angular operation range: the design for \( \lambda = 457 \text{ nm} \) showed good performance over a wavelength range 406–520 nm and an input-angle range 36°–64°. So this technique could be the alliance between the angular/spectral tolerance and large scale production with the simplicity of the structure.

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Table 4. Comparison of simulated (sim.) and experimental efficiencies (meas.) of triplicator at different wavelengths.

| λ (nm) | q − N | Sim. | Meas. |
|--------|-------|------|-------|
| 406    | −17   | 0.185| 0.165 |
|        | −16   | 0.197| 0.190 |
|        | −15   | 0.232| 0.231 |
|        | 0     | 0.011| 0.041 |
| 457    | −17   | 0.250| 0.231 |
|        | −16   | 0.237| 0.240 |
|        | −15   | 0.240| 0.250 |
|        | 0     | 0.005| 0.021 |
| 520    | −17   | 0.268| 0.250 |
|        | −16   | 0.243| 0.240 |
|        | −15   | 0.220| 0.205 |
|        | 0     | 0.001| 0.013 |
| 633    | −17   | 0    | 0     |
|        | −16   | 0    | 0     |
|        | −15   | 0    | 0     |
|        | 0     | 0.596| 0.610 |

Figure 10. Comparison of the theoretical and experimental results. (a) Simulated (blue) and measured (red) diffraction efficiencies for a fixed incident angle and wavelength. (b) Angular dependence of the diffraction efficiencies for a fixed wavelength and orders \( q − N = −17 \) (red), \( q − N = −16 \) (green), \( q − N = −15 \) (blue), and \( q − N = 0 \) (black). Solid lines: theoretical results. Stars: experimental results.

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