Design of high-efficiency dielectric reflection gratings


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We discuss examples of designs for all-dielectric reflection gratings that tolerate high intensity and are potentially capable of placing up to 99% of the incident light into a single diffraction order, such as are needed for contemporary high-power lasers utilizing chirped-pulse amplification. The designs are based on placing a dielectric transmission grating atop a high-reflectivity (HR) multilayer dielectric stack. We comment on the connection between transmission gratings and reflection gratings and note that the grating and the HR stack can, to a degree, be treated independently. Because many combinations of gratings and multilayer stacks offer high efficiency, it is possible to attain secondary objectives in the design. We describe examples of such designs aimed toward improving fabrication and lowering the susceptibility to laser-induced damage. We present examples of the dependence of grating efficiency on grating characteristics. We describe examples of high-efficiency (95%) gratings that we have fabricated by using hafnia and silica multilayers. © 1997 Optical Society of America [S0740-3232(97)01105-8]

1. INTRODUCTION

Contemporary developments of high-power lasers, often based on chirped-pulse amplification, rely extensively on the dispersive properties of diffraction gratings. As noted below, it would be desirable if these reflection gratings could be made entirely of dielectric, rather than metallic, material, in order to minimize energy absorbed and the consequent damage. In this paper we describe some of the concerns related to the design and the fabrication of such all-dielectric gratings.

A reflection grating must incorporate two optical functions: It must combine high reflectivity with diffraction. Conventional metallic gratings combine these two functions in a single conducting surface. The conductivity of the metal forces reflection, while periodic grooves create diffraction. Because metallic gratings owe their reflectivity to conductivity, expressible as a complex-valued refractive index or permittivity, they have a disadvantage for applications that subject the grating to intense radiation: The absorption of radiation causes heating and damage. Transparent dielectric materials have much smaller absorption coefficients than do metals, and therefore optical devices based on dielectric materials have potential for withstanding more intense radiation. Moreover, dielectric structures, when used to create gratings, have unique properties that can offer additional benefits. The present paper describes details of the design of such gratings.

2. DIELECTRIC REFLECTION GRATINGS

Contemporary techniques of interference lithography (or holographic grating fabrication; see Refs. 18–23) offer opportunities for producing a variety of one-dimensional periodically corrugated or grooved surfaces. Such a grating created in a semi-infinite dielectric medium can, for suitably deep and closely spaced grooves, place nearly all of the incident light into one transmitted diffraction order. However, a single air–dielectric interface will not, by itself, produce a grating that has high reflectivity. A second optical element is required to produce high reflectivity. For some purposes, and within appropriate wavelength regions, the reflectivity could be provided by a metallic layer under the dielectric grating. Here, instead, we consider some possibilities for creating purely dielectric devices by utilizing the high reflectivity of a dielectric multilayer stack.

Multilayer stacks of thin (subwavelength-thickness) dielectric films are widely used in the optics industry as antireflection (AR) coatings, polarizers, beam splitters, filters, and highly reflecting mirrors. Rather than relying on conductivity or absorption to produce reflection, multilayer dielectric stacks rely on interference. A succession of (horizontal) planar layers are fabricated with thicknesses such that, for light of a specified wavelength and polarization and incident from above at a given angle, the phases of upward- and downward-traveling waves within each layer reinforce either the upward wave (for reflection) or the downward wave (for transmission (an antireflection (AR) coating)). Commercial optical design software now permits the design of elaborate multilayer structures, simultaneously satisfying a multitude of design goals (e.g., high transmission within one bandwidth and high reflectivity within another bandwidth). However, the range of possible solutions to the multilayer de-
A reflecting multilayer stack can be combined with a dielectric grating in several ways. Multilayer dielectric gratings that have been designed and fabricated for use at x-ray wavelengths typically use hundreds of layer pairs, and the grating is etched through many of these layers (so that each grating ridge comprises a multilayer stack). The fabrication of devices for use at longer wavelengths, from the visible to the infrared, typically follows a different approach. When the goal is a highly efficient reflection grating for optical wavelengths, two types of design have particular interest (see Fig. 1).

First, the grating may be placed onto a substrate and then overcoated with dielectric layers. In principle, the initial grating may be created in photoresist, and the overlying layers may be created with standard vacuum deposition techniques. This procedure does not require an etching step. If the layers remain conformal with the underlying grating, then the structure effectively forms a volume grating. A particular concern with this type of grating is the lack of conformability as the number of layers increases: The flattening of the layers may create a reflecting structure rather than a diffracting structure.

Alternatively, the grating may be placed on top of a multilayer reflecting stack. This type of design allows the multilayer stack to be fabricated independently of the grating. This is the method on which we have concentrated our major efforts.

3. GRATING FABRICATION

The procedures used to fabricate a grating have a significant effect on the theoretical design. In our work the multilayer thin-film stack is used as a substrate for the grating, which we create by using previously described procedures of interference lithography. In brief, we first coat the substrate with a carefully controlled uniform layer of photoresist. Next we expose this photosensitive surface to the stabilized interference pattern at the intersection of two collimated laser beams in a two-arm interference holographic setup (see Fig. 2). Our exposure takes place in an environment of carefully controlled temperature and vibrational isolation, supplemented by an active feedback control of the interference fringes. We develop the latent image to create a corrugated surface, using in situ monitoring to control the profile by terminating the development step at the optimal moment.

Many controllable factors affect the photoresist grating profile: the type and the thickness of the photoresist, the intensity and the duration of the exposure, the type and the strength of the developer, and the duration of the development step. By adjusting these variables, it is possible to obtain groove shapes in the photoresist that vary between nearly sinusoidal and nearly rectangular, with depths and spacings of hundreds of nanometers (comparable with a wavelength of visible light). The inherent flexibility of the several steps and materials offers the designer of gratings a wide range of profiles, although precise connection between the controllable factors and the profile typically involves much trial and error.
though the developed photoresist could serve as the grating,\textsuperscript{19,20,56} it is more fragile than other materials. To create a more robust structure, the photoresist can be overcoated with dielectric material, or, as in our work, the pattern can be transferred to the underlying substrate by using lithographic etching techniques.\textsuperscript{51–56}

4. GRATING MODELING

The theoretical and computational problems associated with dielectric gratings\textsuperscript{16,17,21,24,26,28,39,43,57–68} are much simpler than those occurring with metal gratings.\textsuperscript{38,69–83} Nevertheless, because the grooves are likely to be quite deep (depth comparable with a wavelength $\lambda$ and closely spaced (period comparable with $\lambda$) for high efficiency, it is important to use a rigorous method based on full-vector Maxwell equations. A variety of such methods have been described in the literature.\textsuperscript{84} To provide realistic descriptions of actual gratings, it is essential that we be able to model a variety of grating profiles, not just simple shapes such as sinusoids, rectangles, and triangles.

Most of our results have been based on the multilayer modal method, with $R$- or $S$-matrix propagation, developed by Liao\textsuperscript{85–88} and described by him in great detail. Briefly stated, in this approach we idealize the grating profile as a set of discrete slices, rectangular in cross section, in each of which the material consists of two separate dielectrics. Within each of the two dielectrics of such a horizontal slice, the material is uniform, and hence there exist for the Helmholtz equation simple plane-wave solutions (e.g., sines and cosines of possibly complex arguments). At the vertical interfaces between two regions, appropriate field components must be continuous. As in the simpler cases of fields between infinite parallel plates, this continuity requirement leads to a transcendental eigenvalue equation,\textsuperscript{76,77,89} whose infinite set of solutions provides the arguments of the sine and cosine functions. The constructed modal functions are exact solutions to the Maxwell equations within a slice. Having obtained solutions within a slice, it is then necessary to enforce the continuity equations between layers. The procedure is a generalization to multiple waves of what is required in creating solutions for single waves and multiple thin films.\textsuperscript{34} However, the straightforward multiplication of characteristic matrices, which is used for thin-film modeling, is unsatisfactory for grating modeling, owing to the need to retain evanescent waves. These can introduce growing exponentials that ruin the computation, unless special care is taken, as we do with our $R$- or $S$-matrix method.\textsuperscript{88} As a final step of the computations, the field above and below all grating and dielectric structure is expressed as a Rayleigh expansion, with reflection or transmission amplitudes obtained from the solution to algebraic equations as just described.

As in other rigorous methods, the exact Maxwell equations are transcribed into coupled algebraic equations. The computer codes provide not only efficiencies but also field distributions within the grating. They can be used to model quite general shapes of grating profiles. For predictions of general trends and possible design targets, we use simple parameterized groove shapes (e.g., trapezoids and sinusoids), although it is possible to digitize scanning electron micrograph (SEM) profiles for use as input data to the code.

5. EXAMPLES OF DESIGN CONCERNS

Different grating uses pose different constraints and objectives. For example, in the laser program at the Lawrence Livermore National Laboratory (LLNL) our concerns include the following:

A. High Efficiency

Some of our gratings are intended for use in chirped-pulse amplification pulse compressors. For such applications we require that the diffraction efficiency be as high as possible, over a bandwidth surrounding the nominal laser wavelength (typically 1053 or 1064 nm).\textsuperscript{4} (Efficiency here refers, as is customary in grating theory, to the fraction of the normal-incidence component of the time-averaged Poynting vector that emerges into order $-1$.) The key to high efficiency lies in the grating equation

$$n_d \sin \theta_m = n_a \sin \theta + m \lambda/d$$

relating angle of incidence $\theta$ in a material of refractive index $n_a$ to the diffraction angle $\theta_m$ of order $m$ in a material of refractive index $n_d$ for wavelength $\lambda$ and groove spacing $d$. To ensure highest possible efficiency, we choose the groove spacing so that, in accord with the grating equation, only two orders occur\textsuperscript{90} (specular reflection, of order $m = 0$, and backreflection, of order $m = -1$) and we use the grating in a near-Littrow mount, i.e., the angle of incidence is near the Littrow angle, $\arcsin(\lambda/2d)$, at which reflected order $-1$ travels back along the incidence direction. (Strictly speaking, confining the grating period to allow only two orders is neither necessary nor sufficient for high efficiency. Nevertheless, in practice, this constraint provides excellent results.)

We have used a range of groove spacings. Most recently, we have concentrated on designs with 1480 grooves/mm (groove spacing $d = 676$ nm) to produce gold-overcoated gratings with high efficiency over the wavelength range 800–1100 nm.\textsuperscript{91} For 1053-nm light these gratings have $\lambda/d = 1.56$.

B. Large Size

Some of our gratings, intended for use in large chirped-pulse amplification pulse compressors, are tens of centimeters in diameter (a 100-TW laser system operating at LLNL uses gratings 40 cm in diameter, and a 1-PW laser at LLNL uses 94-cm $\times$ 75-cm gratings). For satisfactory pulse compression, it is important that the wave front maintain high quality across the grating. Therefore we require that the grating efficiency and phase be uniform over a large area.

The requirement for uniform efficiency imposes a requirement for uniform groove profile, implying uniform photoresist exposure. Our holographic procedure exposes the entire surface simultaneously to two large intersecting collimated beams from a krypton-ion laser.\textsuperscript{15} (Alternative methods of exposure raster the interference pattern across the surface.) Because there is unavoidable spatial intensity variation across the large surface of
photoresist, it is essential to have a grating design that is relatively insensitive to such groove variations as result from the nonuniform exposure.

C. High Tolerance for Intense Radiation
Many dielectric materials are available for consideration as thin films in stacks, and the consequent range of refractive indices is appreciable. However, our intended usage with pulses of high peak power, at wavelengths of approximately 1 \( \mu \)m, limits the choice of dielectric materials to high-band-gap oxides, such as silica (SiO\(_2\)) and hafnia (HfO\(_2\)). This severely restricts the range of refractive indices available for designs.\(^{92}\)

Because damage is initiated by deposited radiation energy and because this deposition is dependent on the local value of the (cycle-averaged) electric field, it may be desirable for the grating design to minimize high values of the electric field, particularly at material interfaces where mechanical strength may be weakest.

D. Low Reflectivity of Stack during Exposure
The wavelength of our exposure laser, 413 nm, is well matched to the photoresist. To create the desired interference pattern of 1480 lines/mm, we must expose the photoresist to light incident at approximately 17° (the Littrow angle for 413 nm). It is essential that during this exposure there be no spurious interference patterns, such as occur with reflections from the underlying structure (or from nearby hardware). It is possible to meet this goal by placing an AR coating (or temporary absorbing layer) between the dielectric stack and the photoresist. Such layers add to the complexity of the fabrication and the design. We describe (in Section 7 and beyond) a simpler, alternative procedure.

6. RELATIONSHIP BETWEEN TRANSMISSION AND REFLECTION
Our gratings owe their high efficiency, in part, to the choice of groove spacing and angle of incidence: the spacing \( d < 3\lambda/2 \) and the near-Littrow mount allow only orders 0 and \( -1 \) to propagate. Under such conditions both the single-dielectric transmission grating and the multilayer dielectric reflection grating exhibit regular maxima and minima of diffraction efficiency as a function of groove depth. However, conditions that produce high diffraction efficiency for transmission will produce low diffraction efficiency for reflection. The reason can be understood with the aid of Fig. 3 and the recognition that when a transmission grating directs all downward-propagating incident light into downward-transmitted radiation (light incident at angle \( \theta_i \) and emerging downward at angle \( \theta_t \), say), then the time-reversed situation (radiation from below the grating at angle \( \theta_t \) propagating upward out of the grating into angle \( \theta_i \) will also apply. Figure 3(a) illustrates a low-efficiency grating (basically a transparent layer) atop a multilayer mirror. The undiffracted downward wave (solid arrow) returns from the reflection (dashed arrow) and continues upward, through the transparent grating, to emerge as specular reflection. The opposite case of a high-efficiency transmission grating is illustrated in Fig. 3(b). Here the grating directs all of the incident light into order \( -1 \) (solid arrow). Upon reflection this light will, on passing again through the highly efficient transmission grating, be redirected (dashed curve). This second deflection places the radiation again on the course of specular reflection, and the net effect will be for the grating plus (multilayer) reflector to behave as a mirror. Detailed computations, illustrated below, bear out this intuitive observation.

7. DIELECTRIC TRANSMISSION GRATING
The design of an undercoated multilayer dielectric grating [e.g., Fig. 1(b)] involves two structures: the grating and the multilayer stack. Although the final design involves the joint action of each structure, it is instructive to consider each separately: the surface-relief grating (a dielectric transmission grating) and the multilayer HR stack.

Reliable theoretical descriptions of high-efficiency dielectric transmission gratings date back two decades.\(^{21,24-26,50,57,62,93-96}\) The 1982 paper of Moharam and Gaylord\(^{26}\) presented illustrative transmission efficiencies for gratings whose groove spacing was equal to 1 wavelength (\( \lambda/d = 1 \)) and that were used at the Littrow angle (30°). All such gratings, whatever their groove profile, have only two reflected orders (specular reflection, of order 0, and retroreflection, of order \( -1 \)). If the refractive index is less than 1.5, only these two orders will be propagating orders within the material; for higher refractive indices, orders \( +1 \) and \( -2 \) can propagate within the dielectric, although they will not emerge as transmitted orders into air below the grating. Figure 4 shows the diffraction efficiency of a simple lamellar transmission grating as a function of groove depth and duty cycle (defined here as the ratio of ridge thickness at half-height to grating period).

The transmission efficiency (into order \( -1 \)) exhibits a well-known series of periodic maxima and minima. For a duty cycle of 0.5, the first of these maxima occurs at a depth of approximately 1.7 wavelengths, where it reaches a value of 98%. Efficiencies exceeding 96% are available over a range of depths and duty cycles near these values. (For wavelength 351 nm, a high-efficiency transmission grating with duty cycle approximately 0.5 requires grooves approximately 600 nm deep.)

Many of the features of transmission gratings occur also with metallic reflection gratings. Although the surface boundary conditions of dielectric materials differ from those of conductors, some properties of metallic grat-
ings can be expected to appear for reflecting dielectric gratings. Metallic gratings that allow only two orders and whose profiles have Fourier sine expansions have the general property that their diffraction efficiency depends primarily on the fundamental Fourier coefficient of the groove profile. Thus results obtained for sinusoidal profiles are applicable to lamellar profiles having duty cycle 0.5. It is to be expected, and is seen, that dielectric gratings show a similar insensitivity to details of the groove profile.

The response of a grating depends, often markedly, on the polarization of the incident light. It is possible to achieve high efficiency for either TE or TM polarization. (For TE polarization the electric field is parallel to the grooves; for TM polarization the magnetic field is parallel to the grooves.) In general, high efficiency of a dielectric grating requires deeper grooves for TM polarization than for TE polarization, as can be seen by comparing the TM results in Fig. 5 with the previously shown TE results of Fig. 4.

The efficiency attainable from a simple dielectric transmission grating depends not only on the groove depth but also on the difference between refractive indices in grooves and ridges. The phase difference between waves traveling down through ridges and those passing down through valleys provides the opportunity for interference. As Fig. 6 illustrates (for TE polarization and fixed duty cycle 0.3), the situation is similar to the behavior of an interferometer: A given phase difference (and hence a given diffraction efficiency) occurs for fixed values of the product of depth and refractive-index difference.

8. GRATING BOUNDARY CONDITIONS: TE AND TM POLARIZATION

The practical preference for TE polarization for dielectric gratings contrasts with the case for metallic gratings, for which TM polarization has higher efficiency for shallow grooves. The difference between the two types of grating originates in the boundary conditions of the Maxwell equations, which force continuity across any interfaces of the components of electric and magnetic fields that lie within the surface (the tangential components of \( E \) and \( H \)).

For a grating coated with high-conductivity metal, the interface between the air and the grating is a surface over which the field has simple constraints: The interface must be a nodal surface of the electric field for TE polarization, and it must be an antinodal surface of the magnetic field for TM polarization.

A dielectric grating is more complicated than a metal grating because the boundary condition involves matching the field above and below the surface and not just enforcing a node or an antinode. The boundary condition at the interface can be expressed as continuity of ratios of electric- and magnetic-field components (\( H/E \) is an admittance, \( E/H \) is an impedance). The effect of a multilayer stack need enter the computations of grating fields only as an admittance (or an impedance). Thus it is possible, for fixed incidence wavelength and angle, to treat the multilayer stack independently of the grating; stacks that have the same admittance will impose identi-
cal boundary conditions upon the grating fields and will therefore produce identical behavior. Our concern in the present paper is with high-efficiency reflection gratings, for which the multilayer stack must be highly reflective.

As presented in the text by Macleod (Ref. 34, p. 43), the reflectance at a planar interface between region $a$ and region $b$ is

$$R = |[\eta(a) - \eta(b)][\eta(a) + \eta(b)]|^2,$$

where $\eta(r)$ is the complex-valued tilted optical admittance for region $r$:

$$\eta(r) = \frac{n(r)}{Z_0} \times \left| \frac{\cos \theta_r}{1/\cos \theta_r} \right| \text{ for } \text{TE}$$

$$\eta(r) = \frac{n(r)}{Z_0} \times \left| \frac{\cos \theta_r}{1/\cos \theta_r} \right| \text{ for } \text{TM}.$$ (3)

It is possible to achieve high reflectance at an interface in various ways. The traditional quarter-wave stack has a large real admittance (see Macleod, p. 164) that dominates the unit admittance of air. If the stack has a smaller and complex-valued admittance, then the phase relationship between the two admittances becomes important. When the two admittances have equal magnitudes, then complete reflectance occurs when they are $90^\circ$ out of phase.

9. EXAMPLES OF MULTILAYER GRATING DESIGNS

The basic design problem posed here is to choose the thickness of the uppermost layer and the depth and the shape of the grooves cut into this so that, when combined with a HR multilayer stack, the combination will place almost all of the radiation into the reflected order $-1$. The exact structure of the HR stack is not important for the goal of high efficiency, and there exist many equally high-efficiency designs for multilayer dielectric gratings fabricated from given materials, differing in groove shape, depth, and multilayer thicknesses. This great variety of choices allows us to include subsidiary constraints, such as those listed above. Following are examples of how these objectives can be met.

A. Quarter-Wave Stack

The most common form of a HR multilayer dielectric stack is the ($\text{HL}^n$) stack based on $n$ pairs of high-index (H) and low-index (L) material, each of which introduces one quarter-wave of phase shift at the desired angle. As the number of layers increases, the reflectance approaches closer to unity, within a wavelength band whose width is set by the ratio of refractive indices. With this stack in mind, the simplest high-efficiency multilayer grating designs are based on placing a dielectric-grating atop such a quarter-wave stack. Typically, between 6 and 12 layer pairs prove satisfactory. Either an H or an L layer may be placed at the bottom; the choice may depend on the robustness of the coating procedure. Either an H or an L layer (or some third material) may be made the top layer; in general, the groove depths for high efficiency are inversely proportional to the index of refraction of the material comprising the grating layer.

B. Partially Etched Grooves

It is obviously desirable to have a point design that has relatively little sensitivity to small variations in design parameters, such as layer thicknesses, groove depth, and duty cycle. From a purely theoretical standpoint (disregarding fabrication considerations), robust designs can be obtained by allowing some portion of the top layer to lie beneath the grooves—the grooves are not etched entirely through the top layer. Figure 7 illustrates how grating efficiency is affected by groove depth and by the thickness of the upper layer below the groove for a given duty cycle of 0.3. (The sum of groove depth and subgroove thickness is the total thickness of the dielectric material.) Figures 7(a) and 7(b) show clearly the periodic dependence of efficiency on groove depth. Efficiencies exceeding 99% are predicted for a variety of parameter choices. From

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Fig. 7. Efficiency (order-1 in reflection) versus depth of groove (in micrometers) and top-layer thickness below the groove (in micrometers) for a quarter-wave stack. The grating grooves are lamellar, with 1480 grooves/mm (groove period 677 nm), and the duty cycle is 0.3. The radiation is the 1053-nm wavelength at the Littrow angle (51.2°), with TE polarization. The high-index material is hafnia (index 1.9), and the low-index material is silica (index 1.46). The quarter-waves are defined for the use wavelength and angle. (a) High-index surface layer over ($\text{HL}^7$) stack, (b) low-index surface layer over ($\text{HL}^7$)H stack.
Fig. 7(a) it can be seen that when the surface layer has high index (H on top), one high-efficiency design would be grooves approximately 200 nm deep etched into approximately 400 nm of surface layer (leaving a 200-nm sub-groove thickness). When the low-index material is uppermost, efficient performance requires much deeper grooves than this. Figure 7(b) shows that one high-efficiency design would be grooves approximately 700 nm deep in 900 nm of surface layer (leaving a 200-nm sub-groove thickness). Whereas Fig. 7(a) shows that the efficiency with a high-index grating tends to be either very high or very low, Fig. 7(b) shows that when the grating material is of lower index, there occur designs with intermediate efficiencies.

C. Etch-through Designs

High-efficiency designs can be obtained in which the grooves are either partially or completely etched through the top layer. Designs of the latter type are attractive for ease of fabrication: The etching chemistry can be designed to halt at the interface, so that the groove depth is fixed by layer thickness rather than by careful timing of the etching. Figure 8 shows how efficiency depends on depth and duty cycle, for the two possible choices of upper layer, when the grooves are etched all the way through the top layer.

Figures 8(a) and 8(b) display several noteworthy features. In each case gratings with duty cycle greater than 0.5 exhibit a similar periodic variation of efficiency with duty cycle. To bring out this feature, the range of depths for the figures has been taken inversely proportional to the refractive indices of the top layer: 1910 nm of low-index material (index 1.41) and 1410 nm of high-index material (index 1.91), each having the same optical phase. In each of these cases, the shallowest high-efficiency designs are insensitive to duty cycle. Efficiency exceeds 90% for a range of 50 nm at approximately 330-nm depth for H on top and for a range of 100 nm at approximately 730-nm depth for L on top. Peak efficiencies reach 99% for appropriate choices of depth and duty cycle.

These examples show that, in principle, high-efficiency solutions are obtainable for either H or L as the top layer.
Designs based on etching into the higher-index material require significantly shallower grooves. The final choice between the two possibilities involves practical considerations, such as the ease of etching the material and the damage threshold (expected to be higher for low-index material).

D. Connection with Transmission
From the remarks above, it is to be expected that the designs that produce the highest reflected diffraction efficiency will be those for which the grating interface itself has neither very high nor very low efficiency for diffraction in transmission. Figure 9 demonstrates this conclusion, by showing the transmission efficiency of the grating alone, without underlying multilayer structure, for the designs presented in Fig. 8. The parameter choices that produce either high or low efficiency in transmission are choices that produce low efficiency for reflection.

10. EXAMPLES OF SUPPLEMENTARY CONSTRAINTS
The illustrations presented in Section 9, like numerous similar results in the literature, demonstrate the wide range of parameter choices (e.g., grating shapes) that can meet the primary design objective of high diffraction efficiency. The diversity of solutions offers opportunity for imposing additional requirements upon the design. Here we mention examples of these considerations.

A. Problems with Quarter-Wave Stacks
The quarter-wave stack provides one easily understood possibility for creating a high-efficiency reflection grating. However, in our holographic method it has one drawback. The dielectric stack, intended to be highly reflecting at the use angle of 52° for 1053-nm light, is also highly reflecting near the exposure angle of 17° for 413-nm light. (This light is near the reflectivity maximum associated with a third harmonic of the design wavelength.) Figure 10 illustrates an idealized (dispersionless) model of the reflectance expected for a quarter-wave stack at the use angle of 52° and at the exposure angle of 17°. The exposure conditions nearly coincide with the high reflectance of a third harmonic of the use wavelength.

This undesired reflectance can be diminished by altering various layer thicknesses. Commercial optical design software can provide a variety of alternative stacks, with a range of fabrication difficulty, that can minimize the reflectance (at selected wavelengths) during exposure and maximize the reflectance (at selected wavelengths) during use. However, these designs all require precise thickness control of all the layers.

B. HLL Design
A simple alternative to the quarter-wave design (HL)\(n\) is a (HLL)\(n\) design, comprising quarter-waves of high-index material and half-waves of low-index material. Rather than define the quarter-waves for the use wavelength and angle, we choose a shorter wavelength and normal incidence. We have chosen 830 nm for the stack-design wavelength (a choice that simplifies the monitoring of the layer deposition). Figure 11 shows the (idealized disper-
those obtained with the quarter-wave stack: Both designs have, apart from possible phase differences, the same far-field Rayleigh expansion coefficients $R_m$. However, the two designs differ appreciably in the near-field region within the grating grooves. Because the designs have high efficiency, there is a strong standing-wave pattern of the electric field, with antinodal planes where the electric field is roughly twice the value of a free-space traveling wave. With the quarter-wave design, the enhanced-field regions extend into the surface, where they may cause photoinduced breakdown and damage. With the HLL design, adjustments to the uppermost layer can, while retaining high efficiency, shift the enhanced-field regions to fall within the grooves, where they are less likely to induce damage.

Figure 12 shows, for selected high-efficiency cases of the two designs, the spatial distribution of electric-field magnitude. Both designs have high-index material as the top layer and nonzero thickness of this material below the grooves. In the quarter-wave design [Fig. 12(a)], the electric-field maxima are situated at the interfaces in the multilayer stack and at the edges of the grating. In the HLL design [Fig. 12(b)], the maxima are shifted into the low-index silica layers inside the stack and into the air space between the grating ridges above the stack. Therefore this HLL design has theoretically a higher probability of laser damage resistance. (This particular HLL design improved the field placement by adjusting the thickness of the H layer, thereby giving up the fabrication ease of an etch-through design.)

The gratings are intended to have 1480 lines/mm, for which the Littrow angle is $51.2^\circ$ for our intended wavelength (1053 nm), and have only two propagating orders in reflection.

In principle, high-efficiency gratings can be fabricated with either hafnia or silica as the top (corrugated) layer. The etch chemistry differs for the two materials, and consequently the groove profiles differ. In general, one expects that lower-index material will require deeper grooves to produce high efficiency.

The multilayer stacks were prepared by using local vacuum deposition facilities. We coated these stacks with 500–700-nm-thick layers of photoresist by using a spin coater. After soft-baking the films, we exposed them to 413-nm light in the two-arm interferometer described previously. The latent-image photoresist gratings were developed by using in situ monitoring to ensure that grooves were carried through the photoresist to the substrate. The samples were then submitted to reactive-ion etching at remote facilities. Etches in silica were performed by Rochester Photonics Corp. (Rochester, N.Y.), using a reactive-ion etching system and CHF$_3$/Ar/O$_2$ chemistry. Etches in hafnia were performed at Hughes Aerospace Malibu Research Center (Malibu, Calif.), using an ion-beam etcher with CF$_2$Cl$_2$/Ar chemistry. Following the etching, the photoresist mask was stripped by plasma ashing or acetone rinse.

Figure 13 shows an example of predicted diffraction efficiency (when viewed at the Littrow angle) for a HLL stack with (high-index) hafnia as the uppermost (corrugated) layer. For these computations the top layer was taken to have fixed thickness (350 nm), into which were cut grooves of various depths and widths. (The depth of 350 nm corresponds to grooves cut completely through the hafnia.) The profiles were modeled as trapezoids, which is a good approximation to what we produce [see Fig. 14(a)]. According to these computations, we expect that gratings with efficiency exceeding 95% should be produced for a range of groove shapes and base widths; for
duty cycles of approximately 0.3, efficiency is insensitive to depth once the grooves become 150 nm deep.

We have fabricated several hafnia gratings targeting this design. Figure 14(a) shows a SEM picture of a witness sample of a grating whose efficiency, for 1.064-μm light at TE polarization, was 95% (±1%); the remaining light was observed in zero-order reflection. This is lower than our target value of 99%. From measurements on the SEM, it appeared that the silica layers were thinner than the intended 294 nm. Modeling this grating with silica layers of 260 nm, and a topmost hafnia layer 365 nm thick into which are etched trapezoidal grooves 165 nm deep [see Fig. 14(b)], we predicted an efficiency of 95%.

Damage tests\textsuperscript{16,101} of this grating using 300-fs pulses (at 1053 nm and TE polarization) show visible signs of damage at a fluence of 0.21 J/cm\textsuperscript{2} and massive damage (including damage to the multilayer structure) at 1.25 J/cm\textsuperscript{2}.

When silica is used as the top layer, as in the predictions portrayed in Fig. 15, the grooves must be much deeper than for hafnia to produce comparable efficiencies. The grooves tend to be rectangular, as can be seen in Fig. 16(a). Although these grooves are deeper than those needed for the hafnia grating, silica etches much more easily than does hafnia, so the greater depth does not pose a problem. Furthermore, the etching will slow considerably when the grooves reach the hafnia under the silica, and this provides useful control of the depth. As in Fig. 13, the computations here assume a fixed total thickness of silica (800 nm), into which the grooves are etched. As can be seen, for grooves 600 nm deep there occur high-efficiency solutions that are relatively insensitive to the groove width. Alternatively, given a fixed duty cycle of 0.6, there are high-efficiency solutions that are independent of the groove depth for grooves deeper than 650 nm.

We have fabricated several silica gratings that targeted this design. Figure 16(a) shows a SEM picture of a witness sample of a grating whose efficiency was 94% (±1%); the remaining light was observed in zero order.
In this sample the etching was incomplete and did not reach entirely through the silica. Modelining this grating with silica layers of 260 nm, and a topmost silica layer 800 nm thick into which are cut rectangular grooves 720 nm deep (see Fig. 16(b)), we predicted an efficiency of 95%. We expect that, with optimization of our fabrication process, we will be able to raise the efficiency appreciably. For comparison, the highest efficiency that we observe for gold-overcoated gratings, at 1.06 μm, is 95%.

12. UNIQUE PROPERTIES OF MULTILAYER DIELECTRIC GRATINGS

Because the properties of a multilayer dielectric grating derive from interference rather than from conductivity, such a grating will show pronounced variation of efficiency with wavelength. As with multilayer dielectric stacks used for other purposes, it is possible to have multiple design criteria; a grating may be effective in reflecting a selected band of wavelengths while efficiently transmitting other wavelengths.

The behavior of a multilayer dielectric grating, for any given wavelength, polarization, and angle of incidence, is governed by the phase retardation properties of the multilayer stack and the depth and the shape of the grating grooves. These grating characteristics can be adjusted during fabrication in order to control the distribution of energy among reflected, transmitted, and diffracted beams. The wavelength discrimination inherent in a multilayer stack makes it possible to build gratings that transmit or reflect light with high efficiency within a narrow optical wavelength band. Diffraction efficiency (for specific incident radiation) can be adjusted between 0.01% and 98%, so that a grating can be designed to have nearly any desired efficiency and bandwidth. This extreme optical selectivity, which is not possible with conventional metallic or bulk dielectric transmission gratings, allows a narrow spectral region to be selected to the exclusion of all others.

As we have discussed in Section 5, when the groove spacing is sufficiently small only two orders occur in the air outside a grating. Under these conditions one can design a grating to control the relative energy flowing in four directions. For a near-Littrow mounting, these are specular reflection, direct transmission, retroreflection, and Bragg transmitted diffraction. With an appropriate HR multilayer stack, the reflected diffraction efficiency around a selected wavelength can exceed 99%.

A wide variety of designs are possible for combining dielectric gratings with an underlying multilayer dielectric stack. Many of these designs have relatively slight sensitivity to variations in groove shape and depth. In particular, the variety of high-efficiency designs permits choices based on additional constraints, such as ease of fabrication and resistance to damage.

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