The Leaky Mode Resonance Condition Ensures 100% Diffraction Efficiency of Mirror-Based Resonant Gratings

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***Abstract*—The resonance condition of a leaky mode propagating in a dielectric multilayer, which is supported by a mirror and excited by a free space wave from the cover medium, is simply derived from the phase of the reflection at the mirror and cover interfaces. The leaky mode resonance is used to obtain 100% -1st order diffraction efficiency in a reflection resonant grating by destructive interference in the direction of Fresnel reflection. A number of examples support the validity of this condition for high efficiency and illustrate the usefulness of this intelligible representation of the diffraction phenomena for the synthesis of novel diffractive elements.**

***Index Terms*—Gratings, leaky waves, nonhomogeneous media, resonance, waveguide.**

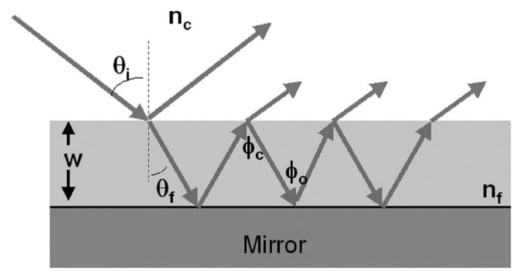

Fig. 1. Single slab dielectric layer of refractive index n_f, width w, based on mirror M. θ_f is the refracted angle in the layer corresponding to the incidence angle θ_i in the cover of index n_c.

I. Introduction

SINCE it has been shown that it is theoretically possible to obtain 100% diffraction efficiency from a resonant grating [1], that more than 99% has been achieved experimentally [2] and that more than 96% is now currently obtained over large areas industrially [3], some design and modeling problems remain open. Whereas zeroth-order resonant reflection from a corrugated (multi)layer waveguide has been widely analyzed from a waveguide standpoint [4], [5], the understanding of resonant diffraction involving a leaky mode is less developed. A 100% -1st order diffraction relies upon the excitation of a leaky mode in a dielectric layer based on a high reflectivity mirror, the grating being a corrugation of one or of both layer sides or an index modulation of the layer. The leaky mode is excited by refraction of an incident free-space wave into the layer. 100% efficiency is obtainable because it is possible to cancel the Fresnel reflection of the mirror-based periodic structure [6]. This highly efficient diffractive effect is not a result of the layer being made of a homogeneous dielectric material. It is a result of the excitation of a leaky mode; therefore, the layer can have a varying index profile or consist of a number of sublayers of different refractive index. Such nonuniform index distribution can lead to useful dispersion properties of the leaky mode such as the fulfillment of the leaky mode resonance over a broad wavelength range. This paper gives a simple way of deriving the leaky mode resonance condition in a multidielectric layer, which is based on a highly reflecting mirror and verifies in a number of different cases that the condition for maximum diffraction efficiency essentially corresponds to the condition of leaky mode excitation.

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II. Leaky Mode Resonance

In a slab layer of constant index n_f and thickness w, which is based on a highly reflective mirror of reflection coefficient $r = |r|\exp(j\phi_0)$, where $|r|$ is close to one, and ϕ_0 is the reflection phase shift on the mirror, covered by a medium of index n_c, usually air, the resonance condition for a leaky mode of order m excited by a plane wave of vacuum wavelength λ under the incidence angle θ_i in the cover is

$$k_0 w n_f \cos\theta_f = m\pi + \frac{(\phi_0 + \phi_c)}{2} \tag{1}$$

where $k_0 = 2\pi/\lambda$ is the vacuum wavenumber, θ_f is the refracted angle in the layer with $\sin\theta_f = (n_c/n_f)\sin\theta_i$, and ϕ_c is the phase of the reflection coefficient of the layer-cover interface upon incidence from the layer side.

It is important to point out here that (1) was obtained under the assumption that the wave field propagates with the temporal t and spatial u coordinates as $e^{j(\omega t - ku)}$, where ω is the angular frequency and $k = (\omega n/c) = (2\pi n/\lambda)$ is the spatial frequency (c is the light velocity in vacuum, λ is the vacuum wavelength, and n is the refractive index of the propagation medium). Had we adopted the $e^{j(ku - \omega t)}$ spatio-temporal dependence, the sign in front of the phase shift terms ϕ_0 and ϕ_c in (1) would be opposite.

Referring to Fig. 1, dispersion (1) determines the values of the w/λ ratio at which a leaky mode resonance of order

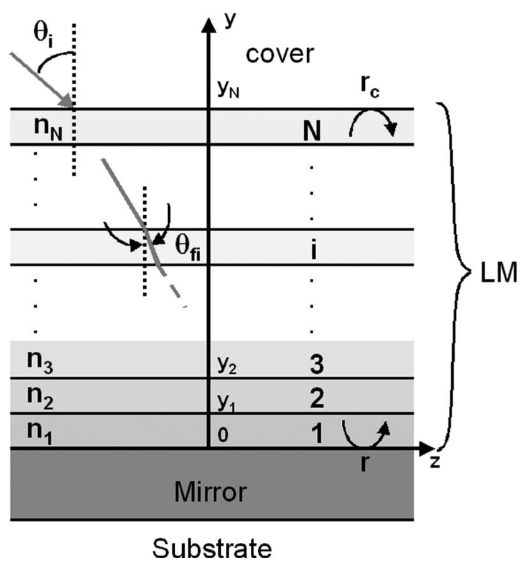

Fig. 2. Cross section of a leaky mode propagating multilayer based on a mirror. $y_1, y_2, \ldots, y_{N-1}$ are the abscissa along y of the interfaces between sublayers $N^\circ 1, 2, \ldots, N$ of index $n_1, n_2, \ldots, n_N$. The abscissa between the interface of the mirror and sublayer N° 1 is 0; that between sublayer N and the cover is y_N.

m occurs under the incidence angle θ_i, the real part of the propagation constant of the mth leaky mode being $k_0 n_c \sin\theta_i$. Equation (1) also gives the real part of the propagation constant $k_0 n_f \sin\theta_f = k_0 n_c \sin\theta_i$ of the leaky modes propagating in a layer of thickness w at wavelength λ. The imaginary part of the propagation constant describing the leakage rate of the leaky mode into the cover and the possible absorption loss of the mirror (if the latter is metallic) is not considered at this stage; it will be considered in the exact grating modeling example of the next section.

It is the real part of the propagation constant which determines the position of the resonance. The mirror is supposed to have zero transmission. If it is made of metal, it will be considered as very low loss and to provide close to 100% reflection modulus with a reflection phase shift ϕ_0. If it is made of a multilayer, it is assumed that the latter is a stack of quarter wave layers of alternating high and low indexes n_h and n_l at the leaky mode wavelength resonance; it provides 100% reflection modulus and a reflection phase shift ϕ_0 of essentially zero or π if the first layer of the multidielectric mirror is of lower or larger index, respectively, than the first sublayer of the leaky mode guiding layer. Fig. 2 illustrates the case of a dielectric mirror, which is composed of quarter wave layers supporting a leaky mode guiding structure LM that is composed of a number N of sublayers of width w_i and index n_i, in which the refracted incident wave propagates under the angle θ_{fi} relative to the normal, the angle θ_{fi} being given as $\sin\theta_{fi} = (n_c/n_i)\sin\theta_i$. z is the propagation axis; the y-axis is normal to layer i and has its origin at the interface between the mirror and the first sublayer of the leaky mode propagating structure. The mirror imposes on the field a boundary condition from where this field will be calculated throughout all sublayers and expressed at the cover interface which imposes a reflection phase shift ϕ_c of zero for the TE polarization, and π for the TM polarization if the incidence angle is smaller than the Brewster angle ($n_c < n_f$ is assumed in this paper, although n_c may also be larger than n_f).

The electric field E_{xi} of a TE leaky mode in sublayer i, which is located within $y_{i-1} < y < y_i$, with refracted angle θ_{fi} and index n_i, is expressed as

$$E_{xi}(y) = A_{mi} \cdot \exp(-j\kappa_i y) + A_{di} \cdot \exp(j\kappa_i y) \qquad (2)$$

where $\kappa_i = k_o n_i \cos\theta_{fi}$ is the projection on y of the k-vector of the plane wave refracted in layer i under the angle θ_{fi}, with $\sin\theta_{fi} = (n_c/n_i)\sin\theta_i$ (if an air cover is considered $n_c = 1$). A_{mi} and A_{di} are the electric field amplitude of the forward and backward y-propagating waves, respectively. The time and z dependence of the form $\exp(j(\omega t - k_0 n_i z \sin\theta_{fi}))$ is left aside.

This paper deals with TE-polarized leaky modes. The field components which are continuous across the interfaces are E_x and H_z. H_{zi} is expressed as

$$H_{zi} = \frac{1}{j\omega\mu_o}\frac{\partial E_{xi}}{\partial y} = \frac{\kappa_i}{\omega\mu_o}\left(A_{di}e^{j\kappa_i y} - A_{mi}e^{-j\kappa_i y}\right). \qquad (3)$$

Applying the continuity conditions at all interfaces $y = y_i (i \geq 2)$ between layers i and $i+1$ of index n_i and n_{i+1} gives the amplitudes A_{di+1} and A_{mi+1} of the backward and forward waves in layer $i+1$ in terms of A_{di} and A_{mi}:

$$\begin{aligned}\begin{pmatrix} A_{di+1} \\ A_{mi+1} \end{pmatrix} &= \frac{1}{2}\begin{pmatrix} M_{i_{11}} & M_{i_{12}} \\ (M_{i_{12}})^* & (M_{i_{11}})^* \end{pmatrix}\begin{pmatrix} A_{di} \\ A_{mi} \end{pmatrix} \\ &= M_i \cdot \begin{pmatrix} A_{di} \\ A_{mi} \end{pmatrix} \end{aligned} \qquad (4)$$

with $M_{i_{11}} = (1 + (\kappa_i/\kappa_{i+1}))\exp(-j(\kappa_{i+1} - \kappa_i)y_i)$ and $M_{i_{12}} = (1 - (\kappa_i/\kappa_{i+1}))\exp(-j(\kappa_i + \kappa_{i+1})y_i)$. Lossless dielectric layers will be assumed; therefore, $M_{i_{22}} = (M_{i_{11}})^*$ and $M_{i_{21}} = (M_{i_{12}})^*$.

At the interface between sublayers 1 and 2 at $y = y_1$, expression (5) relating A_{d2} and A_{m2} to A_{d1} and A_{m1} can be written similarly. However, the presence of the high reflectivity mirror dictates a relationship between A_{m1} and A_{d1} of the form

$$\frac{A_{m1}}{A_{d1}} \cong e^{j\phi_0} \qquad (5)$$

under the hypothesis that the reflection coefficient modulus is close to one. ϕ_0 is the phase shift at the reflection on the mirror. Setting $A_{d1} = E_0$, expression (5) at $y = y_1$ can be written as

$$\begin{pmatrix} A_{d2} \\ A_{m2} \end{pmatrix} = M_1 \cdot \begin{pmatrix} E_0 \\ E_0 e^{j\phi_0} \end{pmatrix}. \qquad (6)$$

At this stage, it is worth pointing out that A_{di+1} and A_{mi+1} actually do not depend on two independent constants A_{di} and A_{mi}, but on a single one E_0, as given by (6). In the last sublayer of order N, the bottom interface at $y = y_{N-1}$ delivers A_{dN} and A_{mN} in terms of A_{dN-1} and A_{mN-1} according to (4). The top interface at $y = y_N$ is between the sublayer of order N and the cover medium which is usually air. However, it can also be a cover medium of refractive index larger than the effective index $n_c \sin\theta_i$ of the leaky mode, or there can be a semireflective structure between the Nth sublayer and the cover medium whose aim may be to provide a larger confinement of the leaky mode field, i.e., a sharper leaky mode resonance. The scope of the present analysis will be limited to the medium adjacent to the Nth sublayer being simply air. At the last interface $y = y_{N-1}$ between sublayers, (6) can be written as

$$\begin{pmatrix} A_{dN} \\ A_{mN} \end{pmatrix} = M_{N-1} \cdot \begin{pmatrix} A_{dN-1} \\ A_{mN-1} \end{pmatrix}. \tag{7}$$

The field coefficients in layer N can be expressed from the field components E_0 and $E_0 e^{j\phi_0}$ at the basis of the structure $(y = 0)$ by matrix multiplication

$$\begin{pmatrix} A_{dN} \\ A_{mN} \end{pmatrix} = M_{N-1}, \ldots, M_2 M_1 \cdot \begin{pmatrix} E_0 \\ E_0 e^{j\phi_0} \end{pmatrix} = M \cdot \begin{pmatrix} E_0 \\ E_0 e^{j\phi_0} \end{pmatrix} \tag{8}$$

where $M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$ has $m_{22} = (m_{11})^*$ and $m_{21} = (m_{12})^*$ in an essentially absorptionless structure.

As from here, the leaky mode resonance condition in the Nth sublayer will be written. It states that the phase shift corresponding to a round trip in sublayer N, taking into account the reflection phase shift at the cover interface at $y = y_N$ and the reflection phase shift at $y = y_{N-1}$ at the interface between sublayers $N - 1$ and N, is an integer multiple of 2π.

The phase ϕ_c of the TE reflection coefficient r_c at the interface $y = y_N$ is zero if the cover index n_c is smaller than n_N; it is π if $n_c > n_N$. If there is a semireflective structure between sublayer N and the cover, the phase of the reflection coefficient should be specifically determined.

Writing the electric field in sublayer N according to (2), with $k_i = k_N$ permits to express the reflection coefficient r_c at $y = y_{N-1}$ with incidence from sublayer N

$$r_c = \frac{A_{dN} e^{j\kappa_N y_N}}{A_{mN} e^{-j\kappa_N y_N}} \tag{9}$$

which by using (9) becomes

$$r_c = \frac{m_{12} \cdot e^{j\phi_0} + m_{11}}{m_{22} \cdot e^{j\phi_0} + m_{21}} e^{j2\kappa_N y_N}. \tag{10}$$

The dispersion equation for a leaky mode simply amounts to equating the phase of r_c given in (10) to zero or to π depending on the relationship between n_c and n_f:

$$\arg\left[\frac{m_{12} \cdot e^{j\phi_0} + m_{11}}{m_{22} \cdot e^{j\phi_0} + m_{21}} e^{j2\kappa_N y_N}\right] - \phi_c = 2m\pi$$

with

$$\phi_{\mathrm{c}} = \arg(r_c) = \begin{cases} 0, & \text{if } n_{\mathrm{c}} < n_{\mathrm{f}} \\ \pi, & \text{if } n_{\mathrm{c}} > n_{\mathrm{f}} \end{cases} \tag{11}$$

where m is the leaky mode order.

ϕ_0 is an important term. It is simply equal to zero or to π in case the mirror is a high reflectivity system of quarter wave layers depending on the relationship between the refractive index of sublayer 1 and the last layer of the multilayer mirror. In case of a metal mirror, ϕ_0 can deviate noticeably from the phase shift of π given by an ideal metal of infinite negative permittivity. Under the hypotheses of weak absorption and large but finite negative permittivity, ϕ_0 is expressed as

$$\begin{aligned} \phi_0 &\cong \pi + \mathrm{arctg}\left(\frac{2\sqrt{-\varepsilon_{mr}}\sqrt{n_1^2 - n_c^2 \sin^2\theta_i}}{n_1^2 + \varepsilon_{mr}}\right) \\ &\cong \pi - \mathrm{arctg}\left(\frac{2\sqrt{n_1^2 - n_c^2 \sin^2\theta_i}}{\sqrt{-\varepsilon_{mr}}}\right) \end{aligned} \tag{12}$$

where $\varepsilon_m = \varepsilon_{mr} - j\varepsilon_{mj}$ is the complex metal permittivity with $-\varepsilon_{mr} \gg \varepsilon_{mj}$ and θ_i is the incidence angle in the cover of index n_c. The phase shift ϕ_0 in the case of a silver mirror at 800-nm wavelength $(\varepsilon_m = -33 + j)$ with a silica layer $(n_1 = 1.46)$ on top and 60° incidence angle θ_i in an air cover $(n_c = 1)$ is 157° instead of π. This implies that the finiteness of the metal permittivity brings the reflected standing wave in the layer adjacent to the metal surface closer to the latter by the amount $\Delta y = ((\pi - \phi_0)/2\kappa_1)$, i.e., 21.7 nm in the present example.

There is another situation where ϕ_0 deviates from zero and π. It is particularly interesting and relates to the case where the incident beam impinges on the mirrored structure from a cover medium different from air; the substrate medium is of refractive index n_s smaller than n_c, and the angle of incidence θ_i in the cover medium is larger than the critical angle $\arcsin(n_s/n_c)$. The very interface between the high index film and the substrate therefore represents a mirror of reflection coefficient of modulus $|r| = 1$. Let us consider Fig. 2 again where the interface between the substrate and the leaky mode propagating structure is located at $y = 0$. Upon total internal reflection between the first sublayer of index n_1 and the substrate of index n_s and under angle θ_{f1}, the reflection phase shift ϕ_0 is known from waveguide optics to be [7] $\phi_0 = 2 \cdot \mathrm{arctg}\sqrt{(n_{\mathrm{e}}^2 - n_s^2/n_1^2 - n_{\mathrm{e}}^2)}$ in the TE case where $n_e = n_1 \sin\theta_{f1} = n_c \sin\theta_i$; therefore, ϕ_0 in this specific case is written as

$$\phi_0 = 2 \cdot \mathrm{arctg}\sqrt{\frac{n_c^2 \sin^2\theta_i - n_s^2}{n_1^2 - n_c^2 \sin^2\theta_i}}. \tag{13}$$

For a given wavelength and a given set of sublayer index and widths, (11) is a dispersion equation to be solved for the angle of incidence θ_i since $\sin\theta_{fi} = (n_c/n_i)\sin\theta_i$, i.e., for the effective index n_{em} of the leaky mode of order m since $n_{em} = n_c \sin\theta_i$. A_{di} and A_{mi} are all given in terms of E_0 which does not get involved in the dispersion equation; therefore, E_0 can be set to the arbitrary value of 1 V/m in the calculations.

The effective index $n_{em} = n_c \sin\theta_i$, where $\sin\theta_i$ is the solution of (11), is not the complex effective index of the leaky modes propagating in the structure; it is its real part which gives the position of resonance. This is the most important information for the design of a close to 100% diffraction efficiency resonant grating [6]. If the resonance width of the leaky mode of order m is a subject of concern, the same analysis can be resumed by replacing $\cos\theta_{fi}$ by the complex variable $\sqrt{n_i^2 - n_{em}^2}$ in all layers and in writing explicitly the boundary conditions for the E_x and H_z field components at the interface between the Nth sublayer and the cover, as described in [8].

Several types of structures can be analyzed as described above: The slab on top of the mirror can comprise a number of alternate low and high index layers in which case there are only two alternating values of κ_i. The structure can also be a graded index layer such as in rugate filters [9].

In a number of cases, the resonant grating structure comprises only two layers on top of the mirror, as for instance in metal-based gratings where the metal base is first coated by a protection layer, like Al_2O_3 in the case of ion-plated silver, then by the dielectric film to be corrugated. Even in the case of a single dielectric film, the corrugation can be considered as a second layer of average permittivity $n_{\text{av}}^2 = ((n_f^2 \cdot \ell + n_c^2 \cdot e)/\Lambda)$ in the TE case, where n_g is the equivalent refractive index of the averaged corrugated layer, ℓ is the grating ridge width, and e is the groove width in a rectangular corrugation of period $\Lambda = \ell + e$. The two-layer case is so often met that it is worth deriving the leaky mode dispersion equation analytically. Inserting the matrix components m_{ij} given in expression (6) into dispersion (11) yields simply

$$\kappa_2 \cdot \tan\left(\kappa_2 w_2 - \frac{\phi_c}{2}\right) + \kappa_1 \cdot \tan\left(\kappa_1 w_1 - \frac{\phi_0}{2}\right) = 0 \quad (14)$$

where w_1 is the thickness of the dielectric layer of index n_1 and $\kappa_1 = k_0\sqrt{n_1^2 - n_c^2 \sin^2\theta_i}$ in direct contact with the mirror and w_2 is the thickness of the top layer (possibly the averaged grating layer) of index n_2 (possibly the equivalent grating index) and $\kappa_2 = k_0\sqrt{n_2^2 - n_c^2 \sin^2\theta_i}$. It can be checked that (14) reduces to (1) if $n_1 = n_2$. Expression (14) is the complete leaky mode dispersion equation containing the reflection phase shift terms unlike in [10, eq. (3)].

Not all multilayer mirrors are composed of quarter wave layers. Close to 100% reflectivity can be achieved by diverse periodic and nonperiodic schemes. A nonperiodic scheme is, for instance, used to confer to the mirror specific dispersion properties; in this case, ϕ_0 is determined numerically. A nonquarter-wave multilayer may be used, for instance, to move the standing wave electric field lobes outside regions where they could lead to optical damage as in femtosecond pulse compressor gratings [11]. In this case, the reflection phase shift is easily calculated. Assuming a multilayer period Λ_m comprising two layers of index and thickness n_{m1}, t_1, n_{m2}, t_2, and ensuring 100% reflection at the first-order of a wave under incidence angle θ_t in the incidence layer medium of index n_t, the multilayer period is $\Lambda_m = t_1 + t_2$. In the general case of a close to 100% reflection dielectric multilayer mirror, which is composed of a periodic set of high and low index layers of nonequal optical thickness, the reflection phase shift ϕ_0 can be calculated from the matrix M_i defined in expression (4).

The field amplitudes $\begin{pmatrix} A_{dnS} \\ A_{mnS} \end{pmatrix}$ at the substrate side of the nth pair of layers of parameters $(t_1, n_{m1}), (t_2, n_{m2})$ are related to the field amplitudes $\begin{pmatrix} A_{dnI} \\ A_{mnI} \end{pmatrix}$ at the incidence side of the same bilayer by the transmission matrix T_n

$$\begin{pmatrix} A_{dnS} \\ A_{mnS} \end{pmatrix} = T_n \begin{pmatrix} A_{dnI} \\ A_{mnI} \end{pmatrix} = \begin{pmatrix} C & B \\ B^* & C^* \end{pmatrix} \begin{pmatrix} A_{dnI} \\ A_{mnI} \end{pmatrix} \quad (15)$$

where $C = [(\kappa_1+\kappa_2)^2 \exp(-j\kappa_1(t_1 - t_2)) - (\kappa_1-\kappa_2)^2 \exp(j\kappa_1(t_1 - t_2))] \cdot (\exp[j\kappa_2(t_1 - t_2)]/4\kappa_1\kappa_2)$ and $B = ((\kappa_1^2 - \kappa_2^2)/4\kappa_1\kappa_2) \cdot 2j \cdot \sin(\kappa_1(t_2 - t_1)) \exp[-j\kappa_2(t_1 + t_2)]$ with $\kappa_1 = k_0\sqrt{n_{m1}^2 - \sin^2\theta_t}$ and $\kappa_2 = k_0\sqrt{n_{m2}^2 - \sin^2\theta_t}$. The next step is the diagonalization of T_n

$$T_n = \begin{pmatrix} B & B \\ \Gamma_1 - C & \Gamma_2 - C \end{pmatrix} \begin{pmatrix} \Gamma_1 & 0 \\ 0 & \Gamma_2 \end{pmatrix} \times \begin{pmatrix} B & B \\ \Gamma_1 - C & \Gamma_2 - C \end{pmatrix}^{-1} \quad (16)$$

where the eigenvalues of T_n are

$$\Gamma_{1,2} = \mathrm{Re}(C) \mp \sqrt{(\mathrm{Re}(C))^2 - 1}.$$

The matrix T_N of a multilayer mirror containing N bilayers is simply obtained from (16) by substituting the Nth power of the diagonalized matrix

$$T_N = T_n^N = \begin{pmatrix} B & B \\ \Gamma_1 - C & \Gamma_2 - C \end{pmatrix} \begin{pmatrix} \Gamma_1^N & 0 \\ 0 & \Gamma_2^N \end{pmatrix} \times \begin{pmatrix} B & B \\ \Gamma_1 - C & \Gamma_2 - C \end{pmatrix}^{-1}. \quad (17)$$

Requiring now that the multilayer is a mirror amounts to setting the condition $|\mathrm{Re}(C)| > 1$, which leads to Γ_i being real and $|\Gamma_1| < 1$ and $|\Gamma_2| > 1$ or conversely. In expression (17), either Γ_1^N or Γ_2^N tends to zero, and the matrix T_N is given by the following proportionality expression:

$$T_N \propto \begin{pmatrix} B(C - \Gamma_1) & B^2 \\ (\Gamma_2 - C)(C - \Gamma_1) & B(\Gamma_2 - C) \end{pmatrix}. \quad (18)$$

The final field amplitudes $\begin{pmatrix} A_{dnf} \\ A_{mnf} \end{pmatrix}$ at the substrate side of the complete multilayer mirror containing N bilayers are related to the field amplitudes $\begin{pmatrix} A_{d1} \\ A_{m1} \end{pmatrix}$ at the incidence side of the same mirror by the transmission matrix T_N. The condition for zero transmission is

$$\begin{pmatrix} A_{dnf} \\ A_{mnf} \end{pmatrix} = T_N \begin{pmatrix} A_{d1} \\ A_{m1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (19)$$

Therefore, the unity-modulus reflection coefficient is

$$r = \frac{A_{d1}}{A_{m1}} = \frac{\Gamma_1 - C}{B} \quad (20)$$

and its phase is

$$\phi_0 = \arg r = \tilde{\varphi} + \kappa_2 t_2 + \frac{\pi}{2}\mathrm{sgn}\left[(\kappa_1 - \kappa_2)\sin(\kappa_1 t_1)\right]$$

where

$$\tilde{\varphi} = \mathrm{arctg} \times \left[\frac{\xi \sin(\kappa_1 t_1 + \kappa_2 t_2) + \zeta \sin(\kappa_1 t_1 - \kappa_2 t_2)}{\sqrt{(\xi \cos(\kappa_1 t_1 + \kappa_2 t_2) + \zeta \cos(\kappa_1 t_1 - \kappa_2 t_2))^2 - 1}} \right] \tag{21}$$

with $\xi = ((\kappa_1 + \kappa_2)^2 / 4\kappa_1\kappa_2)$ and $\zeta = ((\kappa_1 - \kappa_2)^2 / 4\kappa_1\kappa_2)$.

The operation sgn is the signum function. In the particular case where the optical thickness of a pair of layers is λ [corresponding to $\kappa_1 t_1 + \kappa_2 t_2 = \pi$ in expression (21)], the reflection phase shift ϕ_0 at the multilayer is given by the following simpler expression:

$$\phi_0 = \mathrm{arctg} \left[\frac{\sqrt{\frac{(\kappa_1 - \kappa_2)^2}{2\kappa_2\kappa_1}} \left| \sin(2\kappa_2 t_2) \right|}{2\sqrt{\frac{(\kappa_1 - \kappa_2)^2}{2\kappa_2\kappa_1}} \sin(2\kappa_2 t_2) + 1} \right] + \kappa_2 t_2 + \frac{\pi}{2} \mathrm{sgn}(\kappa_1 - \kappa_2). \tag{22}$$

In (21) and (22), it is assumed that the incident layer medium has the same refractive index as the second layer $n_t = n_{m2}$. If the incidence layer medium index n_t differs from the index medium n_{m2} of the multilayer, (23) gives the reflection phase shift φ'_0 to be used in the dispersion (11) or (14) where ϕ_0 is given by either (21) or (22)

$$\varphi'_0 = \mathrm{arctg} \left[\frac{2\kappa_2 \kappa_t \sin \phi_0}{(\kappa_t^2 - \kappa_2^2) + (\kappa_t^2 + \kappa_2^2) \cos \phi_0} \right] \tag{23}$$

where $\kappa_t = k_0 \sqrt{n_t^2 - \sin^2 \theta_i}$, $\kappa_2 = k_0 \sqrt{n_{m2}^2 - \sin^2 \theta_i}$, and θ_i is the incidence angle in the incident layer medium.

In the present electromagnetic problem where the mirror supports a leaky mode propagating structure, the incidence medium of index n_t is the first layer of the leaky mode propagating slab, whose index is noted n_1 and the angle θ_t is θ_{f1} (see Fig. 2). These last formulas are very useful for the use of the present structure synthesis that is based on the fulfillment of the leaky mode excitation condition. The simplified expression was applied to one of the early dielectric pulse compression gratings of the Lawrence Livermore Research Laboratory [13] where the authors make the design of a multilayer mirror at 1053-nm wavelength and 52° incidence angle, so that the latter does not exhibit strong reflection at the grating exposure wavelength. For some practical reason, they choose a multilayer consisting of λ/4 high index layers and λ/2 low index layers, λ being 830 nm and the incidence normal. As a matter of fact, such choice does closely correspond to a multilayer consisting of λ/6 high index layers and λ/3 low index layers under the chosen operation conditions of the pulse compressor (i.e., $\lambda = 1053$ nm and $\theta_i = 52°$ in air). Introducing the data retrieved from the study in [11] into the expression for ϕ_0 gives a reflection phase shift of $-25°$ from a cover medium of index $n = 1.9$.

Using this value of ϕ_0 and the data in [11] concerning the layers and the grating on top of the so-called "HLL" mirror shows that the optimized structure does satisfy the dispersion condition of a leaky mode: The structure is characterized by a 406-nm-thick HfO_2 layer deposited on the "HLL" multilayer mirror under the previous condition ($\lambda = 1053$ nm and $\theta_i = 52°$ in air). The grating is etched with a 236/675-nm duty cycle in the high index layer, which is close to 1.9: The depth is 259 nm. The thickness of the first noncorrugated HfO_2 layer under the grating is then 147 nm. Such a structure satisfies the leaky mode dispersion (12) to within 0.52°.

III. Design of a Resonant Grating of 100% Diffraction Efficiency

As from here, the hypothesis of this paper will be checked in a number of different cases to show its consistency: High, possibly 100% diffraction efficiency is related with the fulfillment of the resonance condition of a leaky mode. Beyond this, however, the diffractive structures described hereafter are also interesting for themselves, in that, they disclose features which are essentially novel.

The consistency test procedure operates as follows: A diffractive structure is first chosen on the criterion of the optical function, and under the conditions, it is expected to perform, for instance, incidence conditions, power level, bandwidth, and layer materials. Then, the structure is submitted to the diffraction analysis and optimization codes of Lyndin based on the true modal [12] or Chandezon *et al.*[13] methods depending on the type of grating technology whether it leads to an essentially binary or smooth profile. The code searches for the structure parameters achieving 100% diffraction efficiency. Then, the corrugation is homogenized and replaced by a uniform noncorrugated layer, the rest of the structure remaining the same.

The homogenization can be of two types: The periodically corrugated region of profile $h(x)$ is replaced by a uniform layer of averaged thickness t_{av} with the same index of the corrugated material in which case t_{av} is given by

$$t_{\mathrm{av}} = \frac{1}{\Lambda} \int_0^{\Lambda} h(x) dx \tag{24}$$

or, in the case of a binary corrugation profile, by a uniform layer having a width equal to the grating depth of average index n_{av} given by

$$n_{\mathrm{av}} = \sqrt{\varepsilon_\ell \cdot \frac{\ell}{\Lambda} + \varepsilon_s \cdot \left(1 - \frac{\ell}{\Lambda}\right)} \tag{25}$$

where ε_ℓ and ε_s is the permittivity of the grating line and of the groove materials, respectively, and ℓ is the width of the grating lines.

Once the corrugated structure has been homogenized, a very shallow virtual grating corrugation is defined at the last interface between the structure and its cover so as to excite its resonances as a numerical experiment. A variation of the period or of the incidence angle permits the scan across the resonance spectrum. Leaky modes are easily identified, as their effective index is smaller than the cover index. The effective index n_{em} of the identified leaky mode of order m is introduced in the

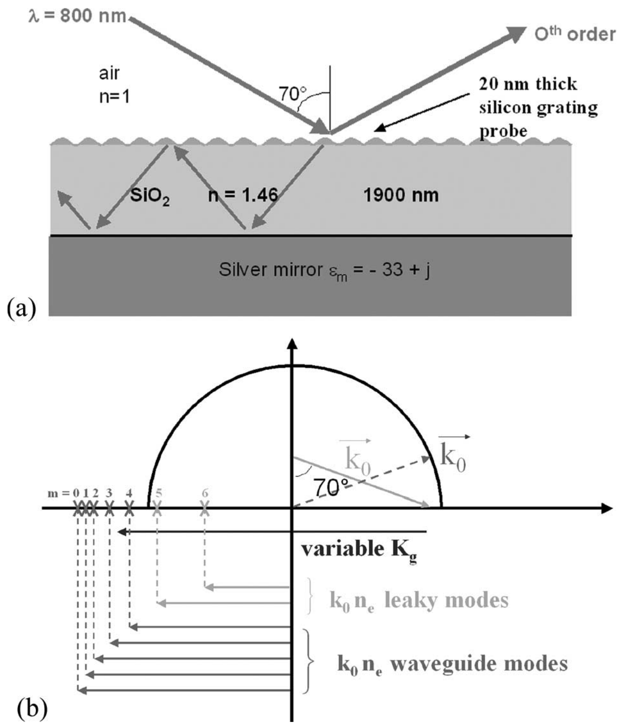

Fig. 3. Example of an SiO_2 slab layer based on a silver mirror with a 20-nm thickness silicon test grating of variable period. (a) Incidence condition: TE polarization under 70° incidence angle. (b) Sketch of the numerical experiment in the reciprocal space with varying grating K_g vector.

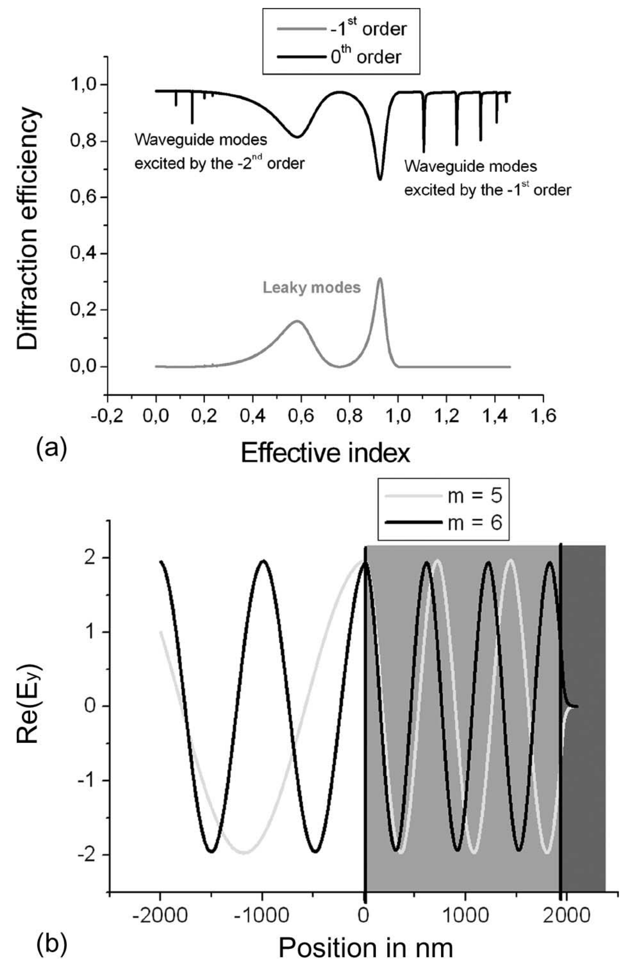

Fig. 4. (a) Diffraction efficiency versus effective index with the structure in Fig. 3. The grating is only 5-nm deep to better display the leaky mode resonances on the first-order. (b) Real part of the electric field for the two leaky modes TE_5 and TE_6.

leaky mode dispersion (11) as $n_{em} = n_c \sin\theta_i$, and it is verified whether the latter is satisfied or how precise it is.

The aim of what follows is to illustrate the numerical experiment of the effective index scan. The structure is sketched in Fig. 3; it is a silver mirror-based dielectric layer composed of SiO_2 of 1.46 index, 1900 nm thickness and a very shallow test silicon grating of 3.5 index at 800-nm wavelength and 20-nm thickness. The reflection phase shift ϕ_0 on the silver mirror is 157.7°, as given by expression (12) where $\varepsilon_m = -33 + j$ at 800-nm wavelength.

An incidence angle θ_i of 70° in air is chosen, and the period Λ is scanned through a domain limited by

$$\Lambda_{\min} = \frac{\lambda}{n_{\mathrm{SiO_2}} + \sin\theta_i} \text{ and } \Lambda_{\max} = \frac{\lambda}{\sin\theta_i}$$

where $\Lambda_{\min}$ is the grating period which would diffract under a grazing direction the first-order of the test grating into the slab layer material (here SiO_2), supposing the latter is semi-infinite, and $\Lambda_{\max}$ is the period which would excite a leaky mode of the structure of effective index zero (the corresponding diffracted beam would be normal to the structure). Fig. 4(a) shows the reflected diffraction efficiency in the zeroth order and the -1st order of the structure under TE incidence versus the effective index variable $n_e = (\lambda/\Lambda) - \sin\theta_i$: The grating depth is only 20 nm to display distinctly the behavior of each mode. Each peak or dip in the reflection curves corresponds to a modal resonance. Those resonances characterized by $n_e > 1$ are waveguide resonances, whereas $n_e < 1$ corresponds to leaky modes leaking into the air cover. The latter are much broader resonances because of the leakage. Their width increases with the decrease of the effective index, since the smaller the effective index, the larger the incidence angle and the smaller the partial reflection at the air boundary.

Fig. 4(b) shows the field profiles in the dielectric layer corresponding to TE leaky modes of effective indexes $n_e = 0.62$ and $n_e = 0.94$. Introducing these effective indexes in dispersion (11) with the corresponding structure parameters in Fig. 3 results in a phase term of about 6π for $n_e = 0.62$ and 5π for $n_e = 0.94$. The effect of the silicon test grating was accounted for in the dispersion equation by an equivalent uniform SiO_2 layer of $(n_{\mathrm{Si}}^2 + 1)/(2n_{\mathrm{SiO_2}}^2)$ times the grating depth, i.e., 62.1 nm.

Fig. 4(a) shows five TE-guided modes corresponding to mode orders $m = 0$ to 4 and two leaky modes corresponding to $m = 5$ and 6 in the leaky mode dispersion equation. This is confirmed in Fig. 4(b) which shows that the dominant mode has $m = 5$ zero crossings in the silica layer, whereas the lower effective index leaky mode has six zero crossings. In the case of a metal of infinite conductivity, the first zero of the electric field would be at the metal surface. The conductivity at optical frequencies is finite ($\varepsilon_{\mathrm{Ag}} = -33 + j$), which leads to a shift of the standing wave interferogram toward the metal surface by the amount $\Delta y = ((\pi - \phi_0)/2\kappa_{\mathrm{SiO_2}})$. The field is maximum at the cover interface.

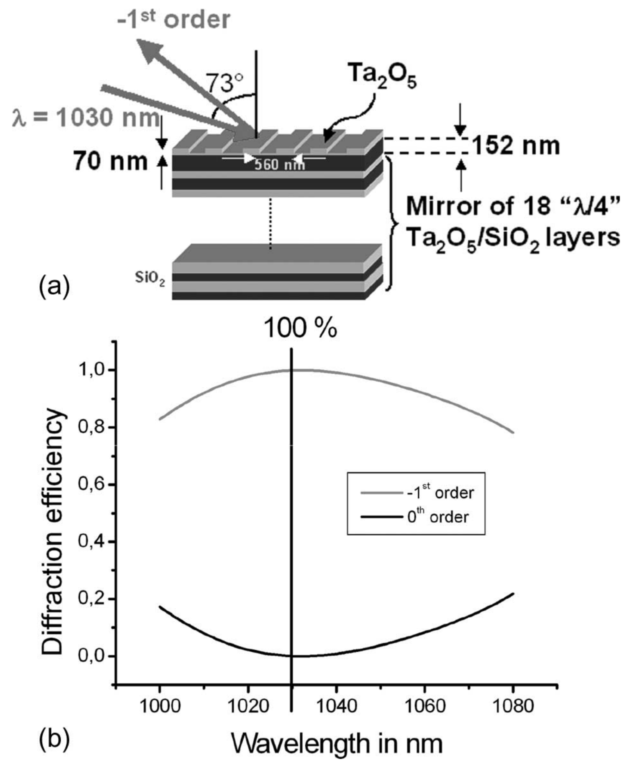

Fig. 5. Example of an experimental structure. (a) Sketch of the structure. (b) Modelized reflection efficiency of first and zeroth orders in the 1–1.1-μm spectral range.

For practical reasons, the TE polarization was preferred since the TM polarization exhibits zero reflection at the Brewster condition, i.e., no leaky mode resonance within the leaky mode range in the neighborhood of the effective index variable $n_e = (n_f n_c / \sqrt{n_c^2 + n_f^2})$.

A number of examples will now be described showing that high, possibly 100% diffraction efficiency can be obtained under the fulfillment of the resonance condition of a leaky mode. The first example of -1st order structure of high efficiency is one for which experimental data are available: More than 99% efficiency was measured [2]. Fig. 5 represents a two-layer slab on a multilayer mirror. The first layer is a fully corrugated high index layer. The objective is to show that the two-layer slab satisfies the leaky mode dispersion equation when optimized numerically for providing 100% diffraction efficiency. The element is aimed at replacing a Lyot filter in a Sagnac laser. The dispersion due to -1st order diffraction must permit the filtering of a longitudinal mode. The diffraction efficiency must be therefore very close to one. The TE incidence angle is 73°. The diffraction angle is 62° with a grating period of 560 nm at 1030-nm wavelength. Fig. 5(a) is the sketch of the structure involving a quarter wave mirror stack made of alternating Ta_2O_5 and SiO_2 layers. The leaky mode propagating structure is an SiO_2 layer with a 50% duty cycle binary grating in a 70-nm-thick Ta_2O_5 layer, as found by Lyndin's optimization code to provide 100% diffraction efficiency [12]. Fig. 5(b) gives the modelized -1st and zeroth-order diffraction efficiency spectra around the nominal 1030-nm wavelength. Homogenized parameters and incidence conditions are introduced in the leaky mode dispersion equation with $\phi_0 = \pi$. One checks that the optimum optogeometrical parameters ensuring 100% -1st order diffraction efficiency satisfy the leaky mode dispersion (11) to within 1.22°.

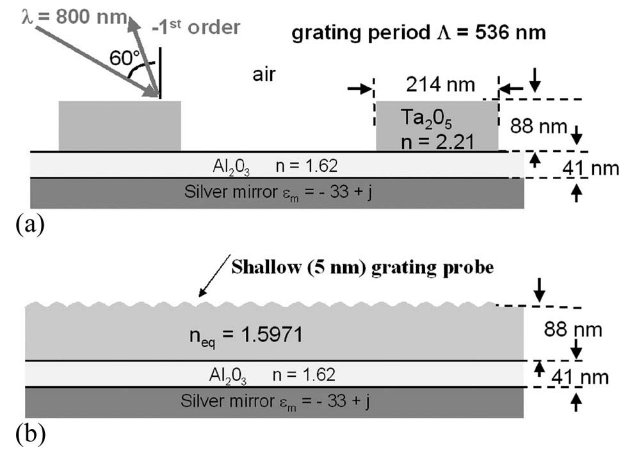

Fig. 6. (a) Optimized silver-based binary grating. (b) Homogenized structure of equivalent index 1.5971 in the grating region with the shallow grating probe for dispersion equation verification.

The second example considered is composed of a first Al_2O_3 dielectric layer of 1.62 index and 41-nm thickness and a second dielectric layer of Ta_2O_5 of 2.21 index and 88-nm thickness based on silver mirror. A diffraction grating is made all through the Ta_2O_5 layer. Submitting the structure to the diffraction optimization code based on the modal method [12], with fixed grating period $\Lambda = 536$ nm, 60° incidence angle, and 800-nm wavelength, leads to 100% -1st order diffraction efficiency with a 214-nm-wide Ta_2O_5 grating lines. The incidence condition imposes a leaky mode effective index of $n_e = 0.627$.

Fig. 6 represents under the resulting structure and the homogenized structure of averaged index of 1.597. Fig. 7 gives the -1st order and zeroth-order diffraction efficiency spectra in the 800-nm wavelength region, which is that of the Ti:sapphire femtosecond lasers. Substituting the parameters of the homogenized structure in the dispersion equation reveals that the latter is satisfied within 1.22° of phase. Such wide bandwidth ($>$ 250 nm) of more than 95% diffraction efficiency is very attractive for sub-100-fs pulses of high energy. The presence of the evaporated Al_2O_3 layer is needed here to protect the silver layer against oxidation during the Ta_2O_5 ion plating process. If another deposition is used as Ion Beam Sputtering for instance, another protection layer can be used (silica for instance) or no protection layer if gold is the structure mirror. The parameters leading to leaky mode resonance will change, but close to 100% diffraction efficiency can similarly be achieved.

As a third example, a similar structure comprising one more layer is considered next. The grating of 187/536-nm duty cycle is made in a photoresist layer of 76-nm thickness on a bilayer of Al_2O_3 of 20-nm thickness and 43 nm of Ta_2O_5. The incidence conditions are the same, and the mirror is silver again. The structure parameters were obtained by Lyndin's optimization code to achieve close to 100% -1st order efficiency.

The homogenization of the resist grating layer leads to the equivalent index of 1.262, considering a resist index of 1.64. Introducing the structure parameters in the dispersion equation shows that the latter is satisfied within $-1.96°$.

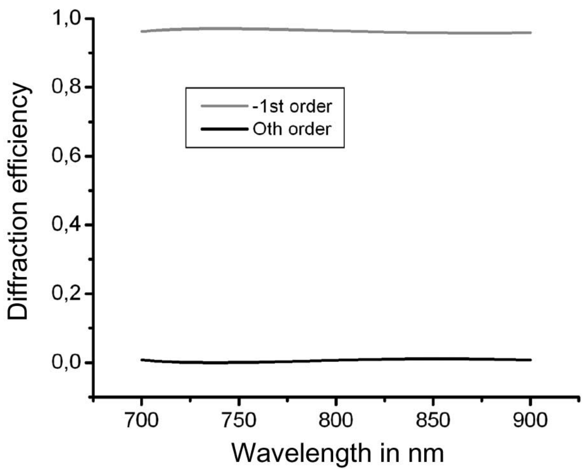

Fig. 7. -1st order and zeroth-order diffraction efficiency spectra in the 800-nm wavelength region of the structure in Fig. 6.

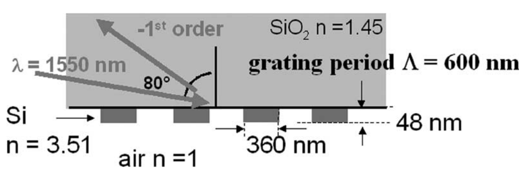

Fig. 8. -1st order resonant grating with total internal reflection for both incident and diffracted waves and segmented very high index leaky mode propagating layer.

As a last example, an original structure is disclosed where the role of the mirror for both incident and diffracted waves is played by a total internal reflection. This implies that the incidence medium has a larger index than the substrate. Fig. 8 sketches a cover medium in silica ($n_c = 1.45$) and "a substrate" of index 1, i.e., air. The leaky mode propagating layer is a binary silicon grating of index 3.51. With a grating period $\Lambda = 600$ nm and incidence angle of 80°, both incident and diffracted waves at 1550-nm wavelength are totally reflected at the base of the fused quartz cover. Here, the dispersion (11) for a single homogenized layer, assuming 0.5 duty cycle, sets a thickness of 51 nm for an average index of 2.58 with the use of the leaky mode of order $m = 0$, effective index of 1.428, and a total reflection phase shift ϕ_0 at the air interface of 23.4° using expression (13). Using the optimization code [12] leads to a thickness of 48 nm, 360/600-nm duty cycle, and equivalent index of 2.795 for the homogenized silicon layer. Substituting these parameters reveals that the dispersion equation is satisfied within 3.8° of phase.

Such grating could be used, for instance, in a monolithic pulse compressor for femtosecond fiber lasers. Silicon as the grating material was considered as an example of very strong dielectric perturbation for checking the statement of this paper in extreme conditions. Practically, almost any grating layer or multilayer could be used instead of silicon.

IV. Conclusion

It was shown in a number of different examples of -1st order resonant reflection gratings that the achievement of close to 100% diffraction efficiency is related with the fulfillment of the condition of leaky mode resonance in the corrugation region. To that end, some novel structures such as high-efficiency wide-band metal-based pulse compression gratings, total internal reflection gratings with incidence in the high index medium layer have been disclosed. The dispersion equation for the leaky modes of a mirror-based structure of arbitrary index profile has been derived with a useful analytical expression for the widely used two-layer structure. Also provided are closed-form expressions for the reflection phase shift against a periodic multilayer mirror. This paper provides an intelligible and direct synthesis tool for improving existing diffraction devices and to generate new optical functions and structures.

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Dr. Parriaux was the Chairman of the 6th ECIO Conference in 1993 and the 7th International Workshop on Waveguide Theory in 1999.