

Theoretical study of the anomalies of coated dielectric gratings

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Abstract. The zero-order diffraction efficiency anomalies of a corrugated dielectric waveguide are studied theoretically in detail. A new and surprising phenomenon is observed: the efficiency changes from 0 to 100 per cent in the vicinity of the excitation of guided waves. The fundamental parameters of the system are found in the case where only one order is propagating and some of their properties are shown. The behaviour of the efficiency curves is explained by a phenomenological theory and a comparison with numerical rigorous results is made.

1. Introduction

Dielectric coatings are often deposited on the top of metallic gratings in order to protect the metal layer from oxidation and to increase the efficiency, most frequently for aluminium gratings working in the ultraviolet. Sometimes they are used on the top of silver gratings operating in the near infrared region.

The presence of a dielectric layer, however, may drastically change the behaviour of the efficiency curves, as it has been pointed out by Palmer [1] for TE polarization and by Cowan and Arakawa [2] for TM polarization.

The influence of a thick dielectric layer on the diffraction efficiency of a blazed aluminium grating has been investigated experimentally by Hutley *et al.* [3] and the results have been confirmed by a rigorous differential formalism [4]. The reason for the appearance of new anomalies in the efficiency behaviour is the excitation of leaky waves [5], supported by the dielectric layer.

On the other hand, corrugated gratings on the top of dielectric waveguides are widely used in integrated optics as input or output couplers [6], filters, demultiplexers, etc. [7]. However, we are unaware of any detailed study of the diffraction efficiency behaviour of three-layer dielectric gratings. The purpose of this paper is to study the anomalies in the efficiency curves linked with the excitation of guided waves from both numerical and phenomenological points of view. The peculiar behaviour of such anomalies is explained by taking into account only the symmetry properties of the system. Up to the phenomenology, the conclusions are valid for any kind of system with a given symmetry which can support guided waves. A total theoretical study of the dependence of the anomaly characteristics on the system

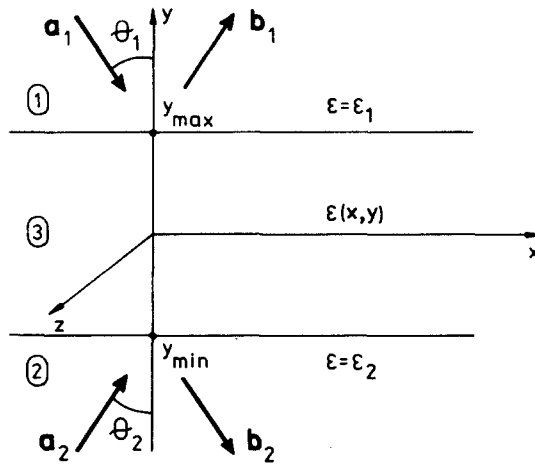


Figure 1. Schematic representation of the three-layer dielectric structure.

parameters for a symmetrical corrugated waveguide is given. The computer code has been developed in the Institute of Solid State Physics (Bulgaria). It is based on a rigorous differential formalism of Chandezon *et al.* [8] for multicoated gratings. A more precise analysis of the advantages and the restrictions of the method is presented in [9].

2. Statement of the problem

Figure 1 represents the most general structure studied in this paper. We consider a system of three lossless dielectric regions 1, 3 and 2 in the rectangular coordinate system $Oxyz$ with refractive indices $\epsilon_1^{1/2}$, $(\epsilon(x, y))^{1/2}$ and $\epsilon_2^{1/2}$ respectively. We suppose that $\epsilon(x, y)$ is periodic in x with a period d and, in general, $\epsilon(x, y)$ is piecewise constant. A plane monochromatic wave with wavelength λ and time dependence $\exp(-i\omega t)$ is incident at an angle θ_1 on region 3 from the side of region 1. We assume that $d \leq \lambda \leq 2d$ so that an interval $\Delta' = (1 - \lambda/d, \lambda/d - 1)$ exists of values of $\alpha = \sin \theta$, where only the zeroth order is diffracted.

For the two fundamental cases of polarization, TE (electric field \mathbf{E} is parallel to the Oz axis) and TM (magnetic field \mathbf{H} is parallel to the Oz axis) we denote by $F(x, y)$ the projection of \mathbf{E} or \mathbf{H} on the Oz axis. Due to the translation invariance on the z axis, the problem is a two-dimensional one.

In order to define the S -matrix it is more convenient to consider that two incident waves illuminate the structure of figure 1: the first with a complex amplitude a_1 under the incidence θ_1 ; the second with a complex amplitude a_2 under the incidence θ_2 such that $\epsilon_2^{1/2} \sin \theta_2 = \epsilon_1^{1/2} \sin \theta_1$. The total field is given by

$$F(x, y) = a_1 \exp [ik(\alpha x - \beta_1 y)] + b_1 \exp [ik(\alpha x + \beta_1 y)] + F_1^e(x, y) \quad \text{for } y > y_{\max}, \quad (1)$$

$$F(x, y) = a_2 \exp [ik(\alpha x + \beta_2 y)] + b_2 \exp [ik(\alpha x - \beta_2 y)] + F_2^e(x, y) \quad \text{for } y < y_{\min}, \quad (2)$$

where $\alpha = \epsilon_1^{1/2} \sin \theta_1$, $\beta_j = \epsilon_j^{1/2} \cos \theta_j$, $k = 2\pi/\lambda$ and $F_j^e(x, y)$ are evanescent fields; $j = 1, 2$.

A particular case of the general system of figure 1 is the array of dielectric cylinders shown in figure 2 (a). In this paper, however, we shall deal mainly with the periodic waveguide of figure 2 (b).

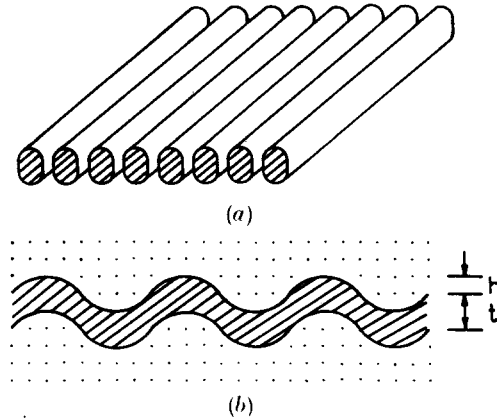


Figure 2. Examples of different kinds of gratings: (a) dielectric cylinders, and (b) corrugated dielectric waveguide.

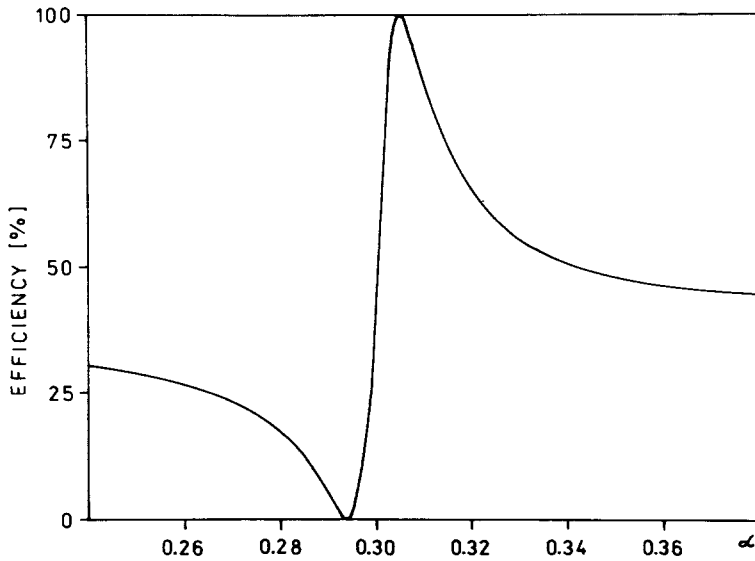


Figure 3. Diffraction efficiency of the zeroth reflected order of the sinusoidal grating, as shown in figure 2 (b). Parameters of the system are: $n_1 = n_2 = 1$, $n_3 = 2.3$, $t = 0.19 \mu\text{m}$, $h = 0.04 \mu\text{m}$, $d = 0.37 \mu\text{m}$ and $\lambda = 632.8 \text{ nm}$, for TE polarization.

The diffraction efficiency $|b_1/a_1|^2$ of the zero reflected order as a function of α , called 'reflectance' $R(\alpha)$ is shown in figure 3 for one of such gratings. The results are obtained using a single precision with 32 bits wordlength. For simplicity we show the results only for TE polarization. It must be pointed out, however, that both the computer code and the phenomenological theory work fairly well for the two fundamental cases of polarization.

The parameters of the corrugated waveguide is chosen in such a way that only one mode would propagate if the interfaces were plane. We see from figure 3 that in the vicinity of the excitation of the guided wave the efficiency changes from 0 to 100 per cent. To our knowledge such peculiar behaviour of the efficiency has not been previously reported. Further we shall demonstrate that this surprising phenomenon is characteristic for the general system of figure 1.

3. S-matrix and the symmetry of the system

3.1. Properties of the S-matrix

If we denote by \mathbf{b} the complex vector

$$\begin{pmatrix} b_1 \beta_1^{1/2} \\ b_2 \beta_2^{1/2} \end{pmatrix}$$

and by \mathbf{a} the complex vector

$$\begin{pmatrix} a_1 \beta_1^{1/2} \\ a_2 \beta_2^{1/2} \end{pmatrix},$$

the S-matrix is defined by the linear relation

$$\mathbf{b} = S\mathbf{a}, \quad (3)$$

where S is a square matrix of size 2 with elements S_{ij} , $i, j = 1, 2$. We consider that the wavelength λ , the shape of the grating profile and the incident n_i are fixed. Therefore the components of the S-matrix are a function of the only variable $\alpha = \sin \theta$. Further we deal with the analytical continuation of $S(\alpha)$ in the complex α -plane at a certain distance from the cut-off and from the Rayleigh anomalies in the domain Ω of the complex plane, containing Δ' .

From (1) and (2) it follows that the S-matrix is invariant by translation in x because the dependence of the incident and the diffracted field in x is of one and the same kind. Energy balance criterion implies that the energies of the incident and the diffracted fields must be equal, when α is real. Therefore S is a unitary matrix:

$$\forall \alpha \text{ real: } S^*(\alpha)S(\alpha) = I. \quad (4)$$

Here I is a unit matrix, $S^*(\alpha) = T_1[\bar{S}(\alpha)]$ is the adjoint of S , the operator T_1 means a transposition and the overbar complex conjugation.

It is well known that if $S(\alpha)$ is analytic and can be continued through the domain Ω of the complex plane, $S^*(\bar{\alpha})$ is analytic too. Since $S^*(\bar{\alpha})S(\alpha)$ is an analytic matrix in Ω , equal to I on a segment Δ' of the real axis, it is equal to I in the entire domain:

$$\forall \alpha \in \Omega, \quad S^*(\bar{\alpha})S(\alpha) = I. \quad (5)$$

Time reversal symmetry implies that the field $\bar{F}(x, y)$ satisfies the Maxwell equations and the boundary conditions. Since ε_i , $i = 1, 2$ is real, from (1) and (2) it follows that in this case α is changed by $-\bar{\alpha}$ and $b_i \rightleftharpoons \bar{a}_i$. Therefore

$$\bar{\mathbf{a}} = S(-\bar{\alpha})\bar{\mathbf{b}}, \quad (6)$$

and from (3) and (5) we obtain

$$S(-\alpha) = T_1[S(\alpha)]. \quad (7)$$

Equation (7) is the matrix representation of the reciprocity theorem.

3.2. Symmetry of the system

Let us now consider the properties of the S-matrix, determined from the different kinds of symmetries of the structures of figure 4: symmetry with respect to a point, symmetry with respect to a vertical axis and symmetry with respect to a horizontal axis.

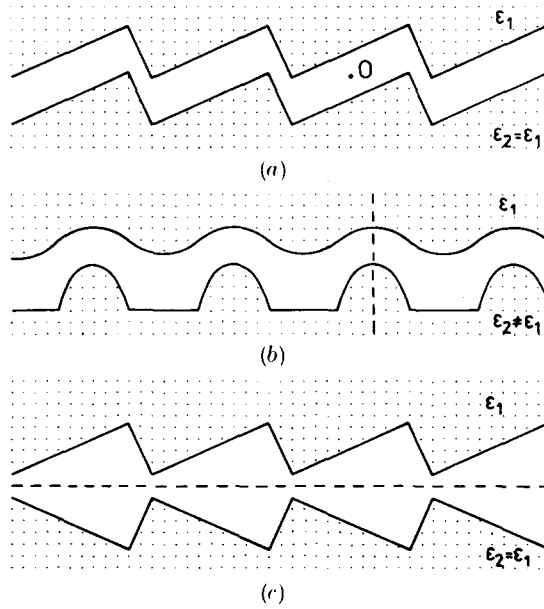


Figure 4. Dielectric corrugated waveguides with (a) symmetry with respect to a centre of symmetry; (b) symmetry with respect to a vertical axis; (c) symmetry with respect to a horizontal axis.

(a) Symmetry with respect to a point (figure 4(a))

Let the origin of the coordinate system be situated at the centre of symmetry. The invariance about the origin implies that $F(-x, -y)$ satisfies the Maxwell equations and the boundary conditions. This is equivalent with the change in (1) and (2) of

$$\alpha \rightarrow -\alpha, \quad a_1 \rightleftharpoons a_2, \quad b_1 \rightleftharpoons b_2 \quad \text{with } \epsilon_1 = \epsilon_2.$$

Applied to the S -matrix, this symmetry gives

$$T_2\{T_1[S(\alpha)]\} = S(-\alpha), \tag{8}$$

where the operator T_2 means the transposition about the second diagonal of the matrix. Using (7), we obtain:

$$T_2[S(\alpha)] = S(\alpha), \tag{9}$$

which leads to $S_{11}(\alpha) = S_{22}(\alpha)$.

(b) Symmetry with respect to the vertical axis (figure 4(b))

Due to the invariance of S -matrix by translation in x , we can take the y axis as an axis of symmetry so that $F(-x, y)$ satisfies the Maxwell equations and the boundary conditions. Now in (1) and (2) we have to change α with $-\alpha$ thus $S(-\alpha) = S(\alpha)$ and using (7) we obtain

$$T_1[S(\alpha)] = S(\alpha). \tag{10}$$

Therefore, the S -matrix is symmetrical about the main diagonal: $S_{12}(\alpha) = S_{21}(\alpha)$.

(c) *Symmetry with respect to the horizontal axis (figure 4(c))*

For this kind of symmetry $F(x, -y)$ is a solution of the Maxwell equations and the boundary conditions. Thus in (1) and (2)

$$a_1 \rightleftharpoons a_2, \quad b_1 \rightleftharpoons b_2, \quad \text{with } \varepsilon_1 = \varepsilon_2.$$

The S -matrix satisfies the relation

$$T_1\{T_2[S(\alpha)]\} = S(\alpha), \quad (11)$$

which implies that S -matrix is symmetrical about the two diagonals: $S_{11}(\alpha) = S_{22}(\alpha)$, $S_{12}(\alpha) = S_{21}(\alpha)$. It is worth noting that this symmetry is the most powerful one, since it includes the properties of the symmetry with respect to the origin and the symmetry with respect to the vertical axis. From this point of view it is impossible to distinguish a grating with both symmetries (a) and (b) from the grating having symmetry (c).

4. Phenomenological approach

Let us consider the corrugated waveguide of figure 2(b). We assume a hypothesis of continuity, i.e. if the grating depth tends towards zero, the field of the corrugated waveguide propagating along the x axis tends to the mode field of the planar waveguide, provided the thickness is above cut-off. The mode field in the outer regions can be represented in the form

$$F^{\text{e}}(x, y) = \sum_n f_n \exp [ik(\alpha_n x + \beta_{1,n} y)] \quad \text{for } y > y_{\text{max}}, \quad (12)$$

$$F^{\text{i}}(x, y) = \sum_n h_n \exp [ik(\alpha_n x - \beta_{2,n} y)] \quad \text{for } y < y_{\text{min}}, \quad (13)$$

where $\alpha_n - \alpha_m = (n - m)\lambda/d$, $\beta_{j,n} = (\varepsilon_j - \alpha_n^2)^{1/2}$ and as usually we assume that $\text{Re}(\beta_{j,n}) + \text{Im}(\beta_{j,n}) > 0$ [10]. In the interval $\Delta' = (1 - \lambda/d, \lambda/d - 1)$ more than one value n_0 of n cannot exist for which $\text{Re}(\alpha_{n_0}) \in \Delta'$. The other α_n are such that if $n \neq n_0$ then $\text{Re}(\alpha_n) \notin (-1, 1)$. By comparing (12) and (13) with (1) and (2) it appears that the mode represents a field containing diffracted waves without an incident wave. The coefficients f_{n_0} and h_{n_0} correspond to the amplitudes b_1 and b_2 . Therefore for $n = n_0$, α_n is a pole of the S -matrix, which we denote by α^p .

In general this entails α^p being a pole of all the elements and of the determinant of the matrix. From (5) it is evident that

$$\det [\bar{S}(\bar{\alpha}^p)] = 0. \quad (14)$$

For the corrugated waveguide of figure 2(b) a pole α^p is close to the real axis because the propagation constant α_n must be real, when h tends to zero. In the domain Ω of the complex plane the coefficients of the S -matrix must have also a zero α_{ij}^z , close to the pole, because in the planar case ($h = 0$) the existence of the pole must be compensated by a zero ($\alpha_{ij}^z = \alpha^p$) [10]. From this fundamental property the coefficients of the S -matrix can be represented in the form:

$$S_{ij}(\alpha) = \Gamma_{ij}(\alpha) [(\alpha - \alpha_{ij}^z) / (\alpha - \alpha^p)]. \quad (15)$$

Assuming that the pole and the zeros are simple and that no other pole or zeros exist in the domain Ω we can expect that $\Gamma_{ij}(\alpha)$ are slowly varying functions even when α is close to α^p and α_{ij}^z . The values of $\Gamma_{ij}(\alpha)$ can be approximated, at least for shallow

gratings, with good accuracy with the reflection coefficient $\zeta(\alpha)$ and with the transmission coefficient of the system without corrugation. The reflectance of the three-layer system, however, is a periodically varying function of the thickness of the middle layer t . We exclude the case of $\zeta(\alpha)=0$ (at half wavelength optical thickness), which requires special analysis.

If $\text{Im}(\alpha^p)$ and $\text{Im}(\alpha_{ij}^z)$ are weak, the arguments of $(\alpha - \alpha_{ij}^z)/(\alpha - \alpha^p)$ undergo a phase-shift of 2π when α crosses the pole-zero domain on the real axis. This is illustrated in figure 5 where the phase variation of b_1 is calculated for the system of figure 3. This result confirms the adequacy of the representation (15).

The unitarity of the S -matrix in the complex plane gives some relations between the zeros. By developing (5) we obtain:

$$\bar{S}_{11}(\bar{\alpha})S_{11}(\alpha) + \bar{S}_{21}(\bar{\alpha})S_{21}(\alpha) = 1 \tag{16}$$

$$\bar{S}_{12}(\bar{\alpha})S_{12}(\alpha) + \bar{S}_{22}(\bar{\alpha})S_{22}(\alpha) = 1 \tag{17}$$

$$\bar{S}_{11}(\bar{\alpha})S_{12}(\alpha) + \bar{S}_{21}(\bar{\alpha})S_{22}(\alpha) = 0 \tag{18}$$

$$\bar{S}_{12}(\bar{\alpha})S_{11}(\alpha) + \bar{S}_{22}(\bar{\alpha})S_{21}(\alpha) = 0. \tag{19}$$

Since $S_{12}(\alpha_{12}^z) = 0$, we deduce from (18) that either $\bar{S}_{21}(\bar{\alpha}_{12}^z)$ or $S_{22}(\alpha_{12}^z)$ must be equal to zero. If $S_{22}(\alpha_{12}^z) = 0$ the left-hand side of (17) would be nil, hence $\bar{S}_{21}(\bar{\alpha}_{12}^z) = 0$. This relation together with (15) gives

$$\alpha_{21}^z = \bar{\alpha}_{12}^z. \tag{20}$$

Similar considerations applied to (16), (19) and (15) lead to

$$\alpha_{22}^z = \bar{\alpha}_{11}^z. \tag{21}$$

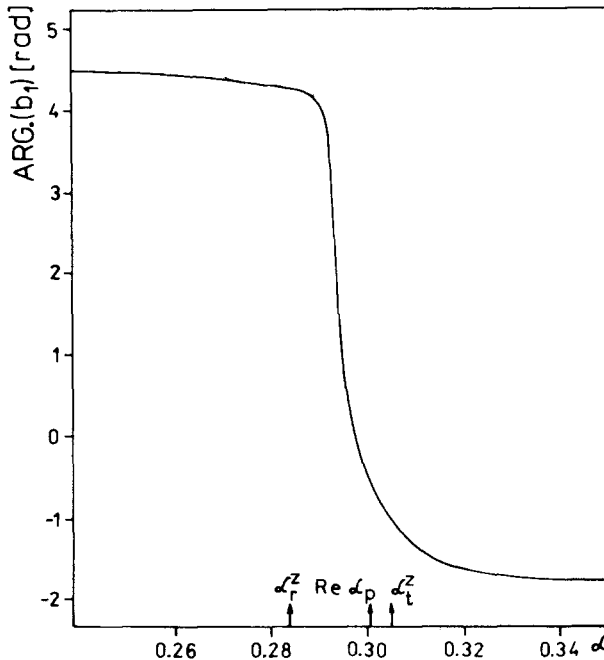


Figure 5. Variation of the argument of b_1 in the vicinity of a resonance, shown in figure 3.

The symmetry of the system imposes further restrictions on the zeros α_{ij}^z . For the symmetry about the centre of symmetry, from (9) and (21) we obtain that the reflection zero is real:

$$\alpha_{11}^z = \bar{\alpha}_{11}^z = \alpha_{22}^z = \bar{\alpha}_{22}^z = \alpha_r^z. \quad (22)$$

In the case of the symmetry about the vertical axis, from (10), (15) and (20) we find that the transmission zero is real:

$$\alpha_{12}^z = \bar{\alpha}_{12}^z = \alpha_{21}^z = \bar{\alpha}_{21}^z = \alpha_t^z. \quad (23)$$

The symmetry with respect to the horizontal axis includes the above kinds of symmetries and thus both the reflection and the transmission zeros are real.

Some sequences for the system of equations (16)–(19) are discussed in [11] with respect to the conservation relations. The phenomenological formula (15) enables us to represent the behaviour of the grating efficiency in the vicinity of the resonance anomaly if the positions of the pole and the zeros are known. In the Appendix a simple geometrical relation between the positions of the pole and the zeros in the complex α plane are given for a system with real zeros. To find them, a Newton iterative method was used and the computer code developed by us had been generalized in order to work for an arbitrary value of α in the complex plane.

Equations (22) and (23) explain the behaviour of the resonance anomaly in figure 3. The corrugated waveguide has a symmetry with respect to the origin and to the y axis, so the reflectance $R(\alpha)$ and the transmittance $T(\alpha)$ are zero at real $\alpha = \alpha_r^z$ and $\alpha = \alpha_t^z$ respectively. If the waveguide is asymmetrical, but possesses a symmetry about the vertical axis (e.g., symmetrical corrugation function), according to (23) only the phenomenon of a zero transmission would occur, because α_t^z is complex. Numerical experiment fully confirms this statement. Figure 6 shows the good agreement between the efficiency curves calculated by the rigorous theory and by the phenomenological formula (15).

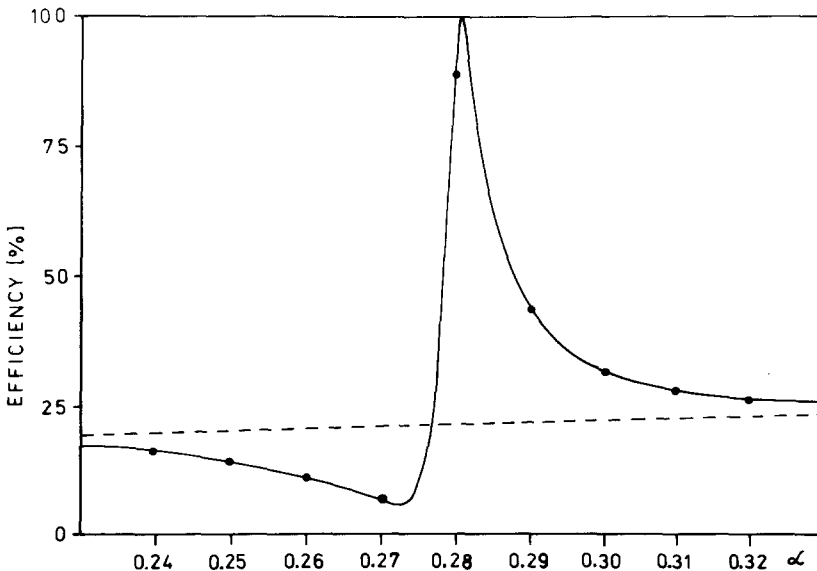


Figure 6. Resonance anomaly of the zero-order efficiency of a three-layer sinusoidal grating near the excitation of the guided wave. The parameters of the waveguide are $n_1 = 1$, $n_2 = 1.6$, $n_3 = 2.3$, $t = 0.1 \mu\text{m}$, $h = 0.02 \mu\text{m}$. The solid line is the calculated curve from the rigorous electromagnetic theory, and the points are the results from (15) with phenomenological parameters $r = 0.2046$, $\alpha^p = 0.286 - i0.0031$, $\alpha_r^z = 0.2874$ and $\alpha_t^z = 0.2808 - i0.00366$.

5. Systematic study of symmetrical corrugated waveguide

The computer codes based on the rigorous electromagnetic theories [12] are unable to give a priori information about the nature of the anomalies. On the other hand we saw in the preceding section that the phenomenological study correctly predicts not only the position but also the shape of the resonance anomaly. The aim of this section is to present the dependences of α^p , α^z , r and R^\dagger on the parameters of the system. In this way the behaviour of the efficiency in the vicinity of the excitation of guided waves is completely determined.

As a particular example we consider a sinusoidal grating of figure 2(b) with a period $d=0.37 \mu\text{m}$, wavelength of the incident wave $\lambda=0.6328 \mu\text{m}$ and refractive indices $n_1=n_2=1$, $n_3=2.3$, so that only the zero-order is diffracted. Figure 7(a) shows the dependence of the phenomenological parameter r on the waveguide thickness t for several groove depth h . With increasing h both r and R decrease (figure 7(b)). The reflectance R is smaller than r since in the investigated case $|\alpha_r^z| < |\alpha^p|$. The investigation of α^p , α_r^z and α_t^z is carried out in the interval of t (figure 8) where no anomaly interaction exists and thus the alteration of r is small. The position of the pole (figure 8(a)) is always close to the point of excitation of the waveguide mode. Without corrugation $\text{Re}(\alpha^p) = \alpha_r^z = \alpha_t^z = \beta/k - \lambda/d$, $\text{Im}(\alpha^p) = 0$ (figure 8(b)) and, of course, in the efficiency curve no anomaly occurs. This represents the well known fact that without corrugation the incident wave cannot excite a waveguide mode.

A trajectory of the pole for several depths of the grating is shown in figure 9. With increasing the depth of the grating the imaginary part of the pole increases, while $\text{Re}(\alpha^p)$ decreases. This is not surprising since the losses of the guided wave, proportional to $\text{Im}(\alpha^p)$, is enhanced by the scattering by the grating. Moreover, figure 10 shows that for small values of h the difference $\Delta = \alpha_r^z - \alpha_t^z$ and $\text{Im}(\alpha^p)$ rise proportional to h^2 . The parameters of the system are independent of the sign of h , thus the linear term must be equal to zero.

Appendix

Let us suppose that for the diffraction system:

- (i) poles and zeros exist,
- (ii) in the investigated domain of parameters the pole and the zeros are simple, and
- (iii) the symmetry provides that both reflection and transmission zeros are real.

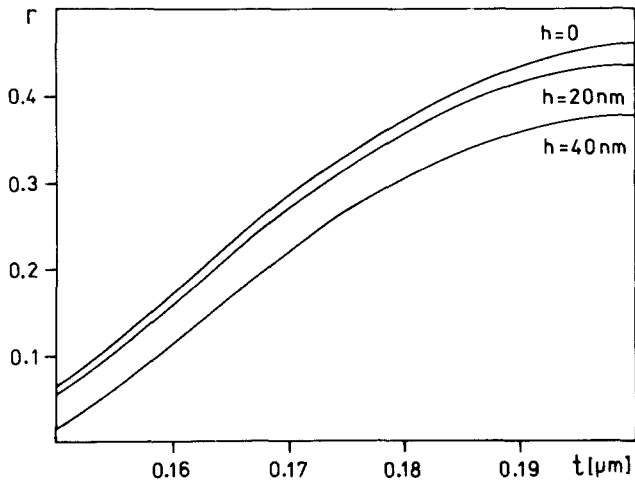
The reflectance and the transmittance of the zero-order are given by

$$R(\alpha) = r(\alpha) \left| \frac{\alpha - \alpha_r^z}{\alpha - \alpha^p} \right|^2, \quad T(\alpha) = \tau(\alpha) \left| \frac{\alpha - \alpha_t^z}{\alpha - \alpha^p} \right|^2. \quad (\text{A } 1)$$

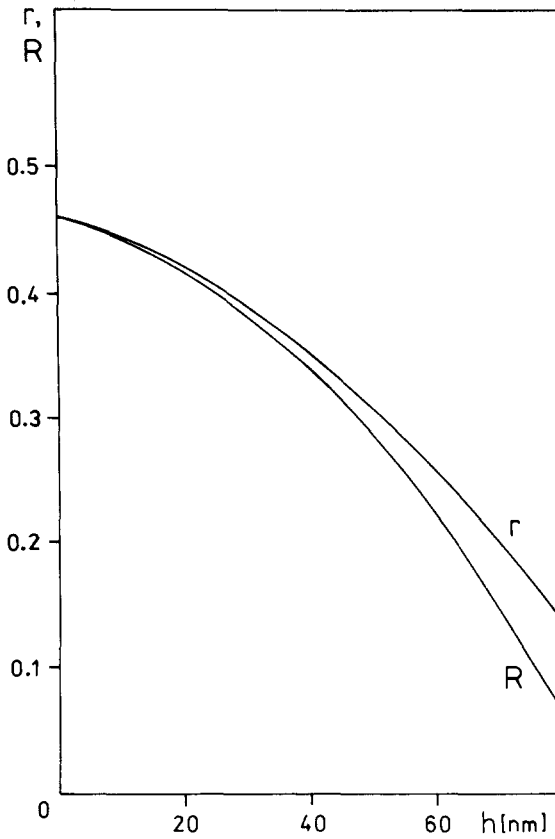
The energy balance on the real axis of α requires that

$$R(\alpha) + T(\alpha) = 1. \quad (\text{A } 2)$$

† The coefficients $r(\alpha) = |\Gamma_{11}(\alpha)|^2$ and $\tau(\alpha) = |\Gamma_{21}(\alpha)|^2$ represent 'phenomenological reflection' and 'transmission' which in the case without anomaly directly correspond to the efficiencies of the zeroth reflected or transmitted order.



(a)



(b)

Figure 7. (a) The parameter r as a function of the waveguide thickness t at a normal incidence. (b) Dependence of r and R on the grating depth h at $\alpha=0$, the waveguide thickness is $t=0.19\ \mu\text{m}$.

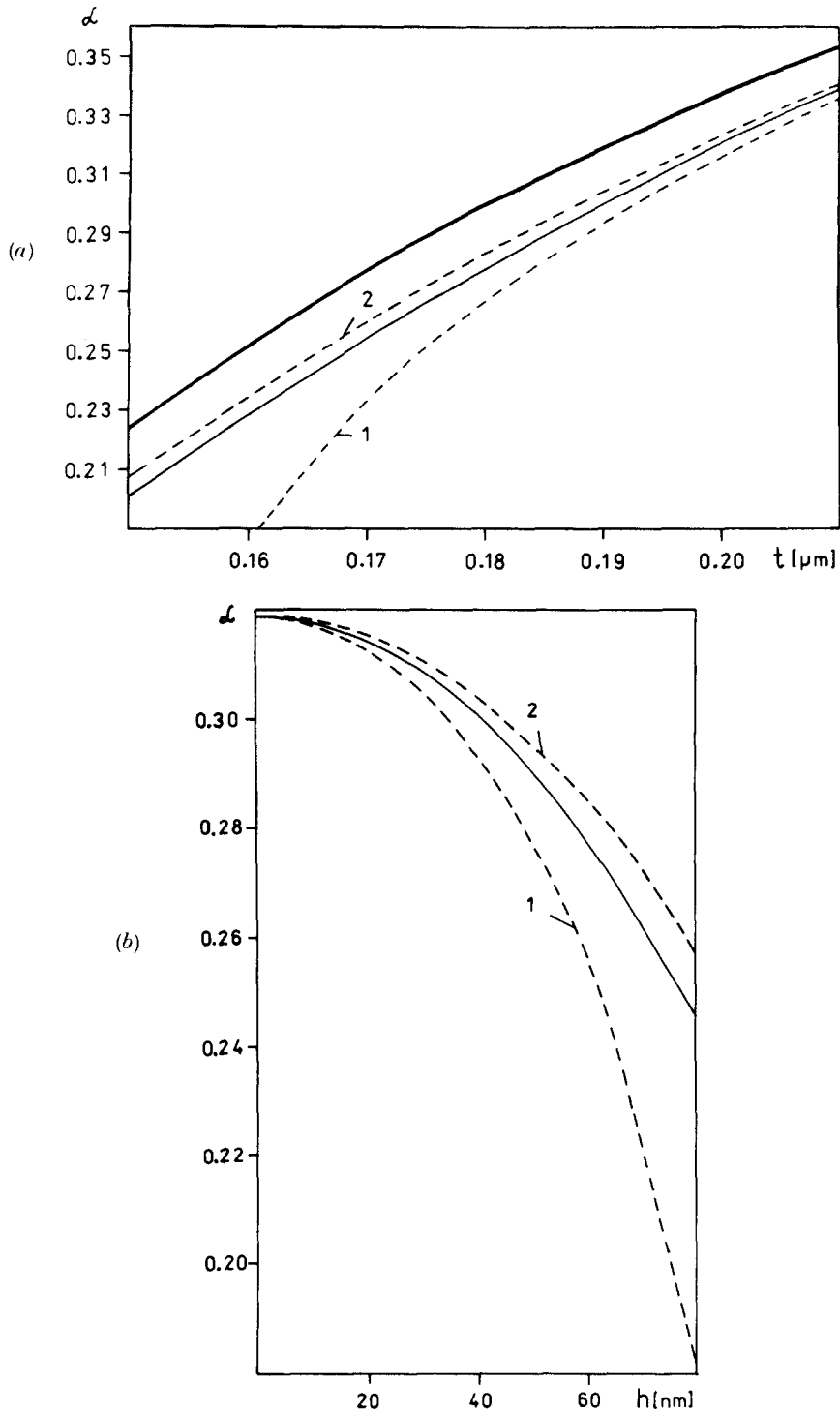


Figure 8. Variation of the real part of the pole (light full line), transmission zero α_t^z (broken line 1) and reflection zero α_r^z (broken line 2), (a) as a function of t for $h=0.04 \mu\text{m}$, and (b) as a function of h for $t=0.19 \mu\text{m}$. The curve $(\beta/k - \lambda/d)$ for the planar system is shown by the bold curve.

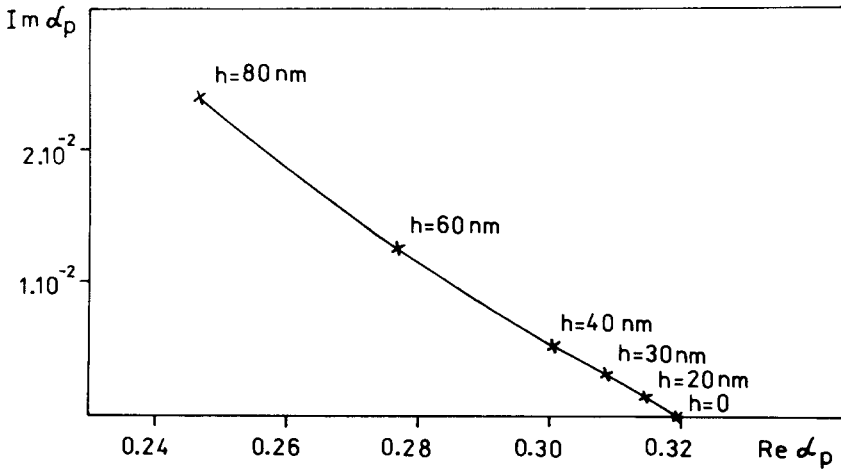


Figure 9. Trajectory of the pole corresponding to a guided wave for a sinusoidal coated grating when the groove depth is varied.

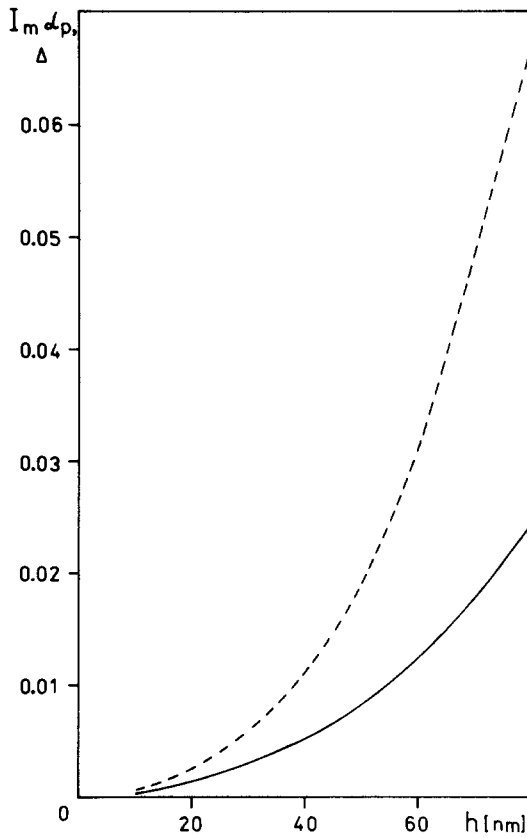


Figure 10. Variation of the distinction between the zeros and variation of the imaginary part of the pole as a function of the groove depth; $t = 0.19 \mu\text{m}$.

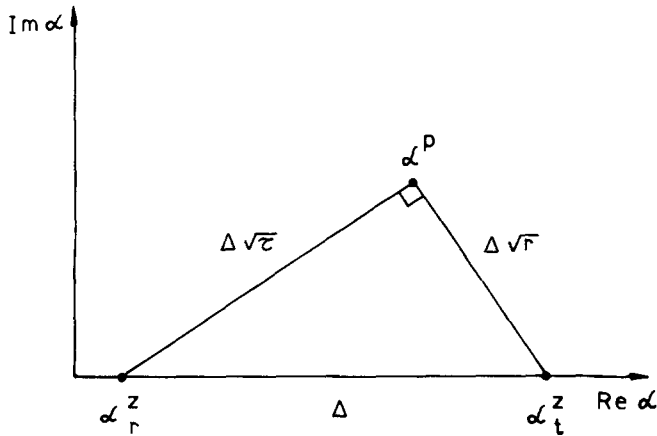


Figure 11. Geometrical relations between α^p , α_r^z , α_t^z , r and τ in the α -complex plane for a system with real zeros.

Since $R(\alpha)$ and $T(\alpha)$ are non-negative,

$$\left. \begin{aligned} \frac{\partial R}{\partial \alpha} \Big|_{\alpha=\alpha_r^z} &= 0, & R(\alpha_t^z) &= 1, \\ \frac{\partial T}{\partial \alpha} \Big|_{\alpha=\alpha_t^z} &= 0, & T(\alpha_r^z) &= 1. \end{aligned} \right\} \quad (A 3)$$

Substitution of (A 1) into (A 3), taking into account the condition (ii) ($r(\alpha) \approx \text{constant}$, $\tau(\alpha) \approx \text{constant}$) yields that the pole and the zeros are located in the apexes of a rectangular triangle (figure 11). This simple geometrical rule enables one to calculate the values of the reflectance and of the transmittance in the domain of anomaly if only the position of the pole and one of the zeros are known.

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