Anomalies of metallic diffraction gratings

L. Mashev* and E. Popov

Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Lenin Boulevard, Sofia 1784, Bulgaria

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A detailed analysis of anomalies of metallic gratings is performed for a large interval of groove depths. Two types of zero of the zeroth diffraction order are distinguished: the Bragg type [Alta Freq. 38, 82 (1969)], exhibited in a Littrow mount for both TM and TE polarizations and localized for flat surfaces at negative imaginary infinity in the complex α plane of the sinus of angles of incidence, and a second type, connected with plasmon–polariton existence on a planar metal–air interface in TM polarization. The trajectories of these zeros are drawn in the α complex plane, revealing some new connections between them.

1. INTRODUCTION

Since 1902, when Wood observed unexpected changes in the spectra of diffraction gratings,[1] this phenomenon, which he called an anomaly, has attracted the attention of physicists. Their constant interest is due to the following main reasons:

(1) It is important for grating users to have smooth, not only high, diffraction efficiency.
(2) Anomalies, namely, the resonance ones, are the linkage between diffraction phenomena and solid-state physics.
(3) New anomalies and new connections between different types of anomalies were discovered recently.
(4) The explanation and rigorous description of grating properties in the anomaly region is one of the most difficult problems for grating theories and thus is one of the strongest stimuli for their development and the best test for their validity.
(5) Currently it is believed that the resonance anomalies play a great role in nonlinear phenomena, surface-enhanced Raman scattering, etc.

Despite the many studies devoted to grating anomalies, the process of discovering new anomalies continues.

The purpose of this paper is to present some new results concerning anomalies on metal relief gratings, to show the existing connections between them, and to reveal their general physical nature. For this purpose a short historical review on the understanding of anomalies is given in Section 2. Some new results about anomalies in the Littrow mount, for both TE- and TM-polarized incident light, are presented in Section 3. In Section 4 our recent results concerning some new types of anomaly in TM polarization, which were published previously,[2,3] are reviewed. In Section 5, a connection between the two entirely different sets of anomalies (that from Section 3 and that from Section 4) is revealed.

In this paper we examine the zeros and poles of a metallic grating with a sinusoidal groove profile supporting only 2 propagating diffraction orders. Similar investigations could be performed if more than 2 orders were propagating, but then it would be more difficult to achieve a simple and clear understanding of the phenomena.

2. HISTORICAL REVIEW

A detailed historical review of diffraction-grating anomalies can be found elsewhere.[4,5] Here we shall outline only the most important results of the investigations that have made possible our present understanding and classification of anomalies. Lord Rayleigh[6] was the first to connect the anomalous behavior discovered by Wood with the threshold (passing off) of higher orders. Fano[7] proposed the resonance character of anomalies. Hessel and Oliner[8] used a new approach to the grating problem to distinguish between threshold and resonance types of anomalies in the case of TM polarization. The latter type is connected with the excitation of a guided wave along the grating surface and is represented mathematically by the existence of a pole α^p ($\alpha = \sin\theta$, where θ is the angle of incidence) of the scattering matrix.[4,5] For the propagation diffraction orders this pole α^p is accompanied by a zero α^z, so that for the plane boundary $\alpha^p = \alpha^z$ and no pole can be observed. Thus a famous phenomenological approach to the resonance anomalies has been developed, resulting in a simple formula for the mth-diffraction-order amplitude a_m:

$$a_m = c_m(h)\,\frac{\alpha - \alpha_m{}^z(h)}{\alpha - \alpha^p(h)}, \tag{1}$$

where c_m, $\alpha_m{}^z$, and α^p are slowly varying functions of groove depth h.

In their later studies Tseng *et al.*[9,10] showed that an anomaly may exist for TE-polarized light, a so-called Bragg-type anomaly (perfect blazing in a Littrow mount[11]), a zero of the zeroth order not connected with threshold or surface wave excitation, but equivalent to a pole of an improper scattering matrix, corresponding to the opposite sign of the incident wave-vector component in direction perpendicular to the grating plane[9] (for more details see Appendix A). Ebesson[12] applied their approach later to TM polarization and confirmed their results experimentally.

The development of rigorous electromagnetic theories[4] makes it possible not only to treat all kinds of gratings numerically in a practical manner but also to predict the appearance of new phenomena. A typical example is the total absorption of light that results from the excitation of a

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plasmon through the negative first diffraction order, which is called Brewster incidence for metallic gratings[13] and was confirmed experimentally.[14]

Using rigorous numerical methods, Maystre *et al.*[15] showed the possibility of non-Littrow perfect blazing. Mashev *et al.*[2,16] recently drew attention to the so-called black-hole effect (an almost total absorption of light by an aluminum grating supporting 2 orders in grazing incidence) and the existence of Brewster incidence in deep gratings.[3] In Refs. 2 and 3 a connection was drawn relating these four phenomena in the complex plane of α: they all are connected with the existence of a plasmon surface wave on a plane metal–air boundary. We discuss this problem in more detail in Section 4 of this paper.

A decade ago a new class of resonances, called cavity resonances,[17,18] which are mode resonances in the grooves of lamellar metal gratings, was discovered for both TE and TM polarizations; such resonances may[17,18] or may not[19] have any influence on the diffraction efficiency, but they are of great importance to surface-enhanced Raman scattering.[19] It is possible that these phenomena are closely connected with the previously mentioned anomalies in the Littrow mount, but this similarity needs further investigation.

3. ANOMALIES IN THE LITTROW MOUNT

A typical example of the dependence of the diffraction efficiency on the groove depth h is presented in Fig. 1 for a perfectly conducting sinusoidal grating. The wavelength ($\lambda = 0.6328\ \mu$m) and the period ($d = 0.5\ \mu$m) are chosen so that only the zeroth and negative first orders are propagating in air.

When h is increased, the efficiency of the specular order

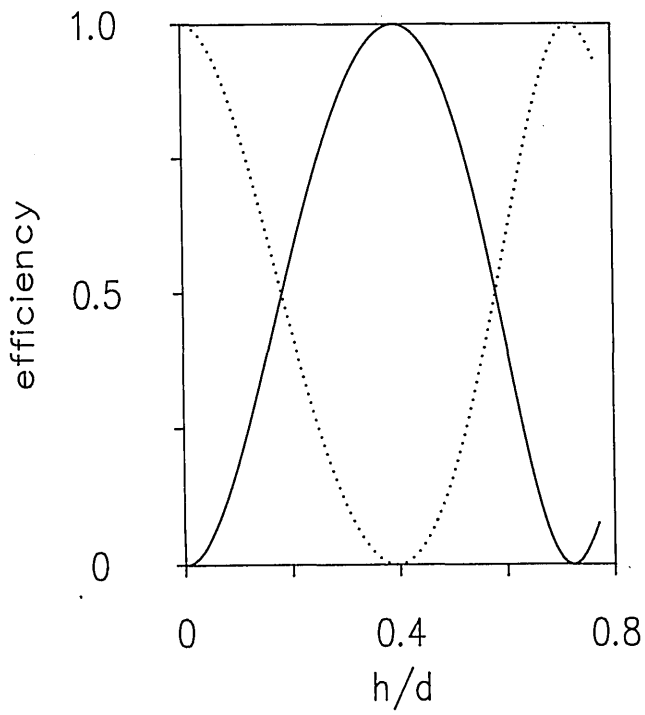

Fig. 1. Groove-depth dependence of the zeroth-order (dotted curve) and negative first-order (solid curve) efficiencies of a perfectly conducting sinusoidal grating in a Littrow mount, with $\lambda/d = 1.2656$ and TM polarization.

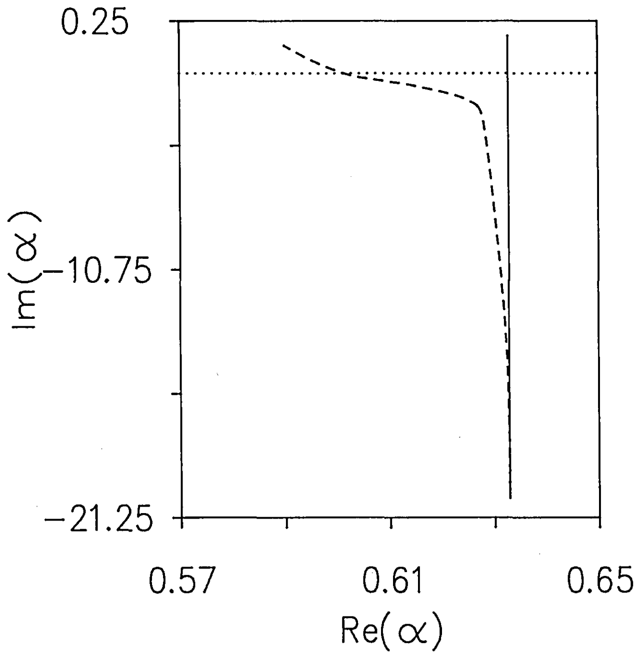

Fig. 2. Trajectory of zeros of the zeroth-diffraction-order efficiency in the complex α plane in the vicinity of a Littrow mount (α_L) for perfectly conducting (solid line) and aluminum (dashed curve) gratings, for $\lambda/d = 1.2656$ and TM polarization. The dotted line represents the real α axis. The corresponding values of the groove depth are given in Fig. 3.

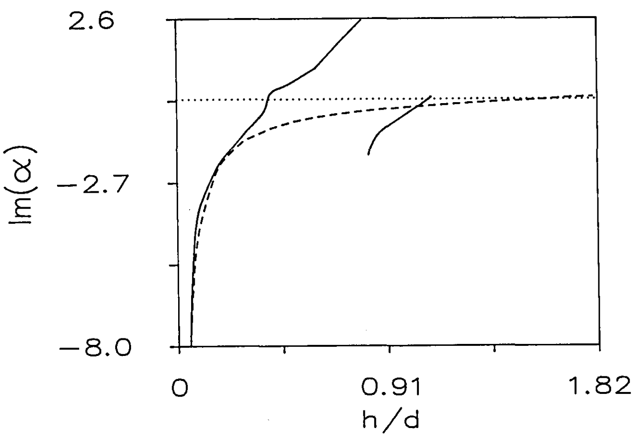

Fig. 3. Imaginary part of the Littrow mount zero of the zeroth diffraction order as a function of the groove-depth-to-period ratio for a perfectly conducting grating and $\lambda/d = 1.2656$. Solid curve, TM polarization; dashed curve, TE polarization. The real part of the zero is equal to α_L. The dotted line represents the real α axis.

passes sequentially through zero values, obtained for $h = h_{L,m}$, $m = 1, 2, 3 \ldots$. These values correspond to the Bragg-type anomaly[9] (Littrow perfect blazing in the negative first order[11]). As was pointed out previously,[9] in the vicinity of $h = h_L$ these zeros (represented by poles of the improper scattering matrix) are shifted in the complex α plane in the direction perpendicular to the real axis. We traced the trajectories of these zeros numerically in a large domain of groove depth (Figs. 2 and 3). In order to trace the zeros far away from the real axis, one must modify the cuts in the complex plane slightly so that the trajectory of the zero does not cross any of them. The first zero $\alpha_{L,1}{}^{z}$ moves along a straight line perpendicular to the real α axis, i.e., passing through the point $\alpha = (\alpha_L, 0)$, where

$$2\alpha_L = \lambda/d. \quad (2)$$

When the groove depth is reduced, $\alpha_{L,1}{}^z$ goes to negative imaginary infinity ($\alpha_{L,1}{}^z \rightarrow \alpha_L - i\infty$). The discovery of this fact has two direct consequences, explaining some already well-known properties:

(1) It directly proves that Littrow zeros of the zeroth reflected order (ZZRO's) constitute a phenomenon entirely different from resonance anomalies, the latter being localized at finite values of $\alpha = \alpha_g$ for a plane interface ($h = 0$), where α_g is the propagation constant of some type of surface wave.

(2) These zeros $\alpha_L{}^z$ can influence the diffraction efficiency only when their imaginary part becomes small enough, i.e., the anomaly exists only for deep gratings.

When the zero is localized far away from the real α axis, numerical experiments show that its imaginary part is proportional to $1/h$ (Fig. 3): whatever the values of the wavelength, the polarization, and the groove profile shape are, the following relations exist:

$$\frac{2\pi}{\lambda}\,\mathrm{Im}(\alpha_{L,1}{}^z)f_{-1} \approx -1,$$
$$\mathrm{Re}(\alpha_{L,1}{}^z) = \alpha_L, \quad (3)$$

where f_{-1} is the negative first Fourier component of the grating profile function $f(x)$,

$$f_{-1} = \frac{1}{d}\int_0^d f(x)\exp(iKx)\mathrm{d}x, \qquad K = 2\pi/d. \quad (4)$$

It must be pointed out that relations (3) are valid even when $\lambda/d > 2$, i.e., $\alpha_L > 1$.

Furthermore, as $h \rightarrow 0$, relations (3) can be satisfied in two different ways:

(1) $\mathrm{Im}(\alpha_{L,1}{}^z) \rightarrow -\infty$. This example is shown in Fig. 3.

(2) $\lambda \rightarrow 0$. We have done a numerical tracing of $\alpha_{L,1}{}^z$ as a function of λ/d for a fixed value of $h = 0.01$ μm, and the results confirm fairly well the validity of Eq. (3). However, when $\lambda/d < 0.666$, both the first and negative second orders appear, and the trajectory of $\alpha_{L,1}{}^z$ crosses the cut in the complex α plane and cannot be traced up to the zero values of wavelength. Andrewartha *et al.*[17,18] found a pole of the first groove mode for lamellar gratings, localized at zero wavelengths for flat surfaces. This pole seems to be quite similar to the Littrow zero discussed above, but further investigations are needed to verify this conclusion. Moreover, usually, when a pole crosses a cut, it is transferred into a ZZRO (see Appendix A), which may explain why Andrewartha *et al.* discussed poles instead of zeros.

As the groove depth increases, $\alpha_{L,1}{}^z$ approaches the real axis, and its influence on the efficiency becomes noticeable. Relations (3) are no longer valid (Fig. 3), and the trajectory of the zero crosses the real α axis for $h/d = 0.394$ in the case of TM polarization and for $h/d = 1.6$ in the case of TE polarization, corresponding to a perfect blazing in the negative first diffraction order.

It should be noted, that, in the case of perfectly conducting gratings supporting only 2 diffraction orders, the efficiency of the zeroth order is symmetrical with respect to the negative first-order Littrow mount, because of the energy-balance criterion and the reciprocity theorem; thus a ZZRO appears exactly for $\alpha = \alpha_L$. This requirement does not hold for real metal gratings. Indeed, numerical results confirm that for an aluminum grating (refractive index $n = 1.378 + i7.616$) the ZZRO is shifted slightly from the Littrow mount (Fig. 2, dashed curve).

When the groove depth is increased further, the imaginary part of $\alpha_{L,1}{}^z$ grows rapidly. We have traced it up to the value of 3 (which is obtained at $h/d \approx 0.8$), because for deeper gratings numerical problems and time consumption make it difficult to go far away from the real axis of α. It must be pointed out that, although the tracing of the zeros and poles for $\mathrm{Im}(\alpha) \gg 1$ cannot have any physical meaning, this tracing is important for establishing connections with other known phenomena. At approximately the same value of $h/d \approx 0.8$ a second zero is found with a negative imaginary part that quickly approaches the real axis along the line $\mathrm{Re}(\alpha) = \alpha_L$ and crosses it for $h/d = 1.08$ (Fig. 3). This cross point corresponds to the second ZZRO efficiency as a function of the groove depth.

4. NON-LITTROW ZERO OF THE ZEROTH DIFFRACTED ORDER

In our previous papers[2,3] we performed a rigorous numerical tracing of the poles and zeros of the zeroth order in a large domain of h/d ratios (ratios as large as 1.4). This tracing enables us to predict the existence of new anomalies and to draw simple connections among them and other already known phenomena. The following considerations are valid for an aluminum grating with a complex value of the refractive index $n = 1.378 + i7.616$. In Fig. 4 the trajectories of the pole (bold curve) and the zero (thin curve) of the zeroth reflected order are given in the complex α plane. A vertical dashed line indicates the cut of χ_0, defined by the equation $\chi_0{}^2 = 1 - \alpha^2$.

For small h/d ratios the pole α^p is associated with surface plasmon excitation. As the groove depth increases, the imaginary part of α^p also increases, corresponding to the increase in the diffraction losses of the surface wave as it propagates along the grating boundary. When the cut is crossed, the pole is converted into a zero. Although the position of the cut is in some limits arbitrary, it always lies above the real α axis; thus, independent of the cut position, the pole is always transferred into a zero. This transition is similar to the transfer of the pole corresponding to the plasmon surface wave into a Brewster-incidence zero, the transfer taking place when the imaginary part of the substrate refractive index is reduced from an infinite value to zero.[5] When the groove depth is increased further, the imaginary part of the zero decreases, and its trajectory crosses the real axis in a point, denoted by $\alpha_{N1}{}^z$, that appears at $h/d = 0.3828$, corresponding to non-Littrow perfect blazing. This phenomenon, discovered by Maystre *et al.*,[15] is associated, for the case of a perfectly conducting substrate, with a diffraction efficiency of 100% in the negative first order.

The second cross point of the curve, denoted by $\alpha_G{}^z$, appears at $h/d = 0.69$ and is exhibited in grazing incidence.

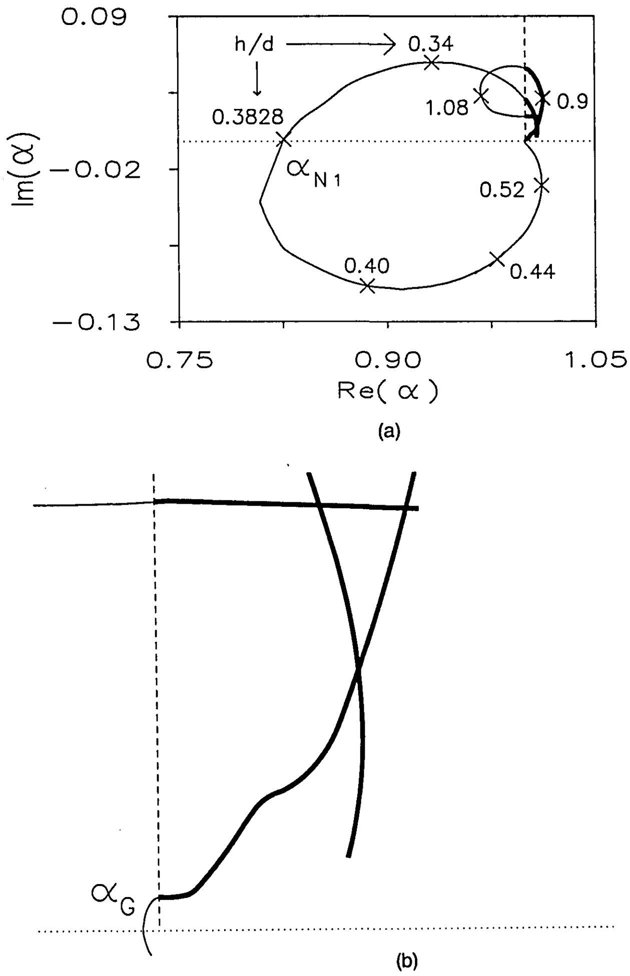

Fig. 4. (a) Trajectory of the pole (bold curve) and the zero (thin solid curve) of the zeroth diffraction order in the complex α plane of an aluminum grating for different h/d values. The cut of χ_0 is indicated by a vertical dashed line, and the real α axis is indicated by a horizontal dotted line. (b) 15× magnification in the vicinity of the point (1, 0).[3]

For a sinusoidal aluminum grating for the same groove-depth values the efficiency in the negative first order is less than 10^{-3} in the entire interval of angles of incidence (the so-called antiblazing effect of gratings.[20] Thus a peculiar phenomenon occurs: a grating supporting 2 diffraction orders acts as a black hole.[16]

As h increases the trajectory of the zero crosses the cut again and is transferred into a pole. In the region of $h/d \in (0.8, 1.4)$ a second loop in the trajectory is formed. These loops correspond to heretofore unknown forbidden gaps in the plasmon dispersion curves, which are not connected with the minigap regions resulting from the interaction of plasmons, propagating in the opposite directions.[21] The decrease of the imaginary part with h in the region of the loops may be connected with the decrease in the diffraction losses in the air.

It is well known[4,5] that the periodical corrugation of the surface leads to the multiplication of the poles of the scattering matrix with the period of the grating. A detailed view of the pole–zero structure in the complex α plane in the vicinity of the point (0.2656, 0) is given in Fig. 5. The trajectory of the pole is symmetrical to that in Fig. 4 with respect to $\alpha = \alpha_L$. There are two principal differences between the two figures:

(1) The trajectory of the pole in Fig. 5 is a piecewise one. Crossing the cut, the pole, which is due to the plasmon excitation through the negative first diffraction order, vanishes, contrary to the situation shown in Fig. 4, in which the pole is transferred into a zero.

(2) The pole in Fig. 5 is accompanied by a zero (for the reasons discussed in Section 2). For perfectly conducting gratings the pole and the zero are symmetrical with respect to the real α axis[4] because of the energy-balance criterion.

When the pole vanishes as it crosses the cut, the zero that lies on the other side of the real axis (where there is no cut) does not disappear. The trajectory of the zero crosses the real axis in four points:

(1) For shallow grooves (h/d = 0.1) the real zero $\alpha_{B1}{}^z$ corresponds to the so-called Brewster incidence, discovered by Maystre and Petit.[13] It is situated in the region where only the zeroth order is propagating, and it leads to a total absorption of incident light.

(2) For $h/d = 0.38$ the second real zero $\alpha_{N2}{}^z$ is symmetri-

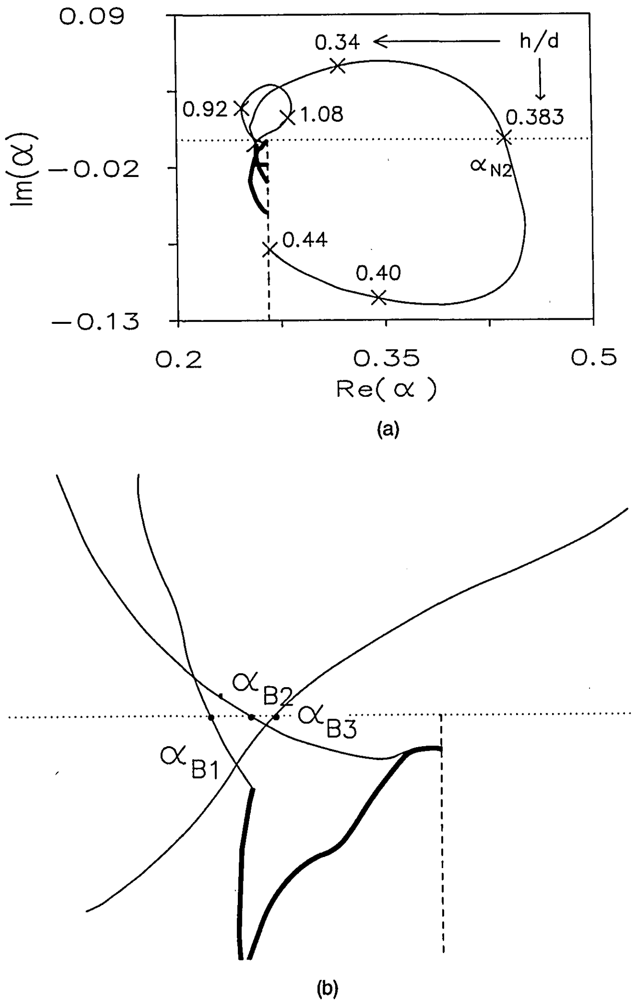

Fig. 5. The same as in Fig. 4 but in the vicinity of the cut of χ_{-1} defined by Re(α) = 1 − λ/d.[3]

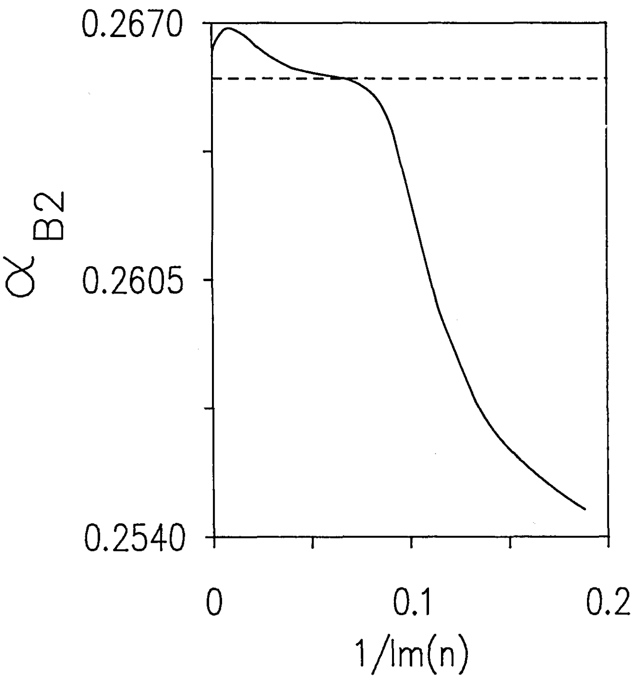

Fig. 6. Location of the second Brewster zero α_{B2} as a function of the imaginary part of the substrate refractive index. The negative-first-order cutoff is shown by a dashed line.[3]

cal to $\alpha_{N1}{}^z$ with respect to the Littrow mount and corresponds to a second non-Littrow perfect blazing for perfectly conducting gratings.[15,22] The values of h/d for which $\alpha_{N1}{}^z$ and $\alpha_{N2}{}^z$ appear are quite close to the value for which the Littrow zero is real. This fact is important to the results given in Section 5.

(3) With a further increase in the groove depth the trajectory of the zero crosses the cut and vanishes. This can be explained easily, at least for perfectly conducting gratings: at the other side of the cut only the zeroth order is propagating, and the existence of a zero without a pole is forbidden by the continuity requirement and the law of energy conservation on the real α axis. As h increases, a pole appears again, and it is accompanied by a zero. As can be predicted by the continuity requirement, the trajectories of the pole and the zero start at the cut. For a perfectly conducting substrate the trajectory of the zero crosses the real α axis at a point $\alpha_{B2}{}^z$ in the region where 2 orders are propagating; thus a third non-Littrow perfect blazing is found to exist that lies near the cutoff of the negative first diffraction order. As the imaginary part of the substrate refractive index n_S is reduced to the real metal values, this cross point is moved toward the cutoff (Fig. 6), and for $\text{Im}(n_S) < 15$ the zero lies to its left-hand side, where only the zeroth order propagates. Thus a total absorption of incident light occurs for deep gratings, too ($h/d = 0.8$).

(4) As can be expected, the existence of the second loop in the pole trajectory for high values of $h/d > 1$ leads also to a new loop in the trajectory of the zero, which crosses the real axis again for $h/d = 1.2$ at a point $\alpha_{B3}{}^z$, corresponding to the third Brewster effect. It is worth noting that the three values of the Brewster angles of incidence in the case of an aluminum grating lie quite close to one another [see Fig. 5(b)].

After this paper was prepared, one of the authors (E. Popov) communicated with Nevière,[23] who obtained independently some of the results presented here. Nevière used a computer code based on the integral formalism, whereas our calculations were performed by the method of Chandezon *et al.*[24] Nevière did a tracing of non-Littrow zeros in the complex α plane for groove-depth-to-period ratios as large as $h/d = 0.72$; his results are in excellent coincidence with our results. Also, Nevière did a numerical tracing of the Littrow zero in the interval $-13 < \text{Im}(\alpha_L{}^z) < 1.5$; again, his results are in good agreement with our results, which are presented in Section 3 above.

5. INTERACTION OF ZEROS

In a previous paper[2] we showed that for shorter wavelengths ($\lambda/d < 1$) the first loop in the zero–pole trajectory (Fig. 4) lies above the real axis and $\alpha_{N1}{}^z$, $\alpha_{N2}{}^z$, $\alpha_{B2}{}^z$, and $\alpha_G{}^z$ do not exist. At $\lambda/d = 1.08$ the loop touches the real axis and two real zeros appear ($\alpha_{N1}{}^z = \alpha_G{}^z$ and $\alpha_{N2}{}^z = \alpha_{B2}{}^z$). When λ/d increases, these two couples are split, $\alpha_G{}^z$ moves toward grazing incidence, and $\alpha_{B2}{}^z$ approaches the negative first-order cutoff. Breidne and Maystre[22] investigated the spectral dependence of $\alpha_{N1}{}^z$ and $\alpha_{N2}{}^z$: their deviation from the Littrow mount decreases as the λ/d ratio increases.

For $\lambda/d = 1.48$ the three zeros $\alpha_{N1}{}^z$, $\alpha_{N2}{}^z$, and $\alpha_{L,1}{}^z$ merge into one another. In Fig. 7 the trajectories of the zeros discussed in Sections 3 and 4 are given in the complex plane for $\lambda/d = 1.56$. A rejection and an exchange of the identities of the curves take place. Such a phenomenon is usually characteristic for pole trajectories but not for zeros. Moreover, the two zeros discussed in Section 4 are, in a peculiar way, connected with a pole, corresponding to the plasmon

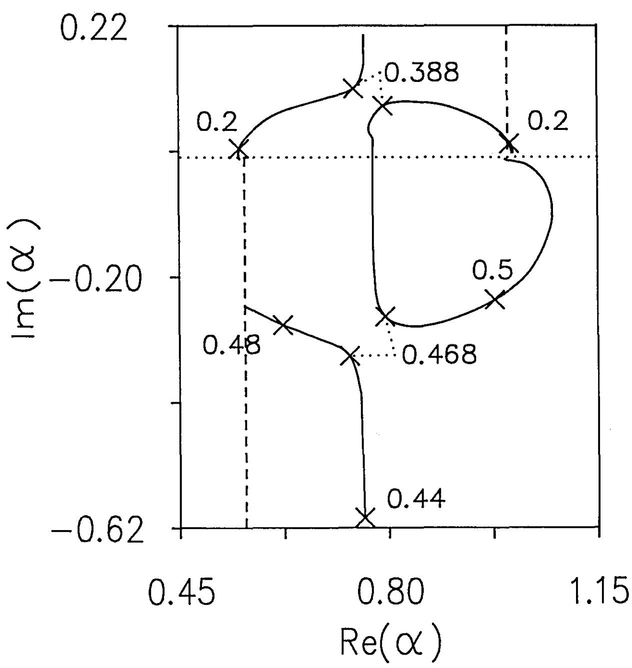

Fig. 7. Trajectories of the zeros (solid curves) of the zeroth-order efficiency of aluminum grating in the complex α plane for different values of h/d, which are indicated by crosses. The horizontal dotted line corresponds to the real axis, and the vertical dashed lines correspond to the cuts of χ_0 and χ_{-1}. $\lambda/d = 1.56$, TM polarization.

excitation, but the Littrow zero is not connected with any surface wave. This contradiction can be explained by taking into account the considerations of Appendix A: the zeroth-order zeros, independent of their origin, correspond to the quasi-resonance, i.e., poles of the improper scattering matrix lying on one and the same improper Riemann sheet. Thus a splitting can be expected in the cross points of the trajectories of the zeros if these cross points correspond to one and the same value of the groove depth, as they do in the investigated case. The last requirement is quite important, and it explains why there is no splitting of the curves in Figs. 4 and 5.

There are some direct consequences of the results presented in Fig. 7:

(1) As a result of the splitting but not of an overlapping of zeros, a single real zero is observed rather than a triplet.

(2) Non-Littrow zeros α_{N1}^z and α_{N2}^z (Refs. 16 and 22) exist only in the spectral region $1.08 < \lambda/d < 1.48$, whereas two other phenomena, connected with α_G^z and α_{B2}^z, exist in the larger interval $1.08 < \lambda/d < 1.98$.

APPENDIX A

It is well-known that a zero in a given diffraction-order efficiency is connected with the existence of a pole of the scattering matrix (i.e., solution of the dispersion relation) lying on an improper Riemann sheet. These improper sheets exist because of the ambiguous character of diffraction efficiency as a function of complex α: there is an arbitrariness in the choice of the sign of χ_m, defined by

$$\chi_m{}^2 = 1 - (\alpha + m\lambda/d)^2, \qquad m = 0, \pm 1, \pm 2, \ldots, \qquad \text{(A1)}$$

and the scattering matrix elements have different values for one and the same α but different signs of χ_m.

Let us investigate in detail the consequences of this ambiguity in the case of a zero α_0^z of the zeroth reflected order having an amplitude a_0^d. The change of the sign of χ_0 is equivalent to the exchange of the incident and reflected zeroth orders (positive χ_0 represents a wave propagating along the positive direction of the axis perpendicular to the grating surface and vice versa). The proper choice of the sign of χ_0 requires that the incident wave (with amplitude a_0^i) propagate toward the grating surface and that the diffracted wave propagate away from the grating.

If, for a given value of $\alpha = \alpha_0^z$, the zeroth reflected order has a zero ($a_0^d = 0$) with a nonzero incident wave (namely, $a_0^i = 1$), the formal exchange of a_0^d with a_0^i resulting from the improper choice of the sign of χ_0 leads to the existence of a diffracted wave with amplitude $\tilde{a}_0^d \equiv a_0^i = 1$, without an incident wave ($\tilde{a}_0^i \equiv a_0^d = 0$), where the tilde over the amplitude denotes the improper sign of χ_0. Thus a pole of the improper scattering matrix $\tilde{S}$ exists:

As far as $a_0^d = 0$, then,

$$S_{00}(\alpha_0^z) = 0, \qquad \text{(A2)}$$

where S_{00} is the element of the scattering matrix corresponding to the interaction between zeroth incident and reflected orders: $a_0^d = S_{00}\, a_0^i$. Then S_{00} in the vicinity of the point α_0^z can be represented as

$$S_{00}(\alpha) = q(\alpha - \alpha_0^z) \qquad \text{(A3)}$$

if it is assumed that α_0^z is a simple zero. On the other hand, an amplitude of the mth diffraction order is given by

$$a_m{}^d = S_{m0} a_0{}^i = \frac{S_{m0}}{S_{00}} a_0{}^d. \qquad \text{(A4)}$$

After the change of the sign of χ_0, a_0^d begins to behave as the incident wave amplitude $\tilde{a}_0^i$, i.e.,

$$\tilde{S}_{m0} = \frac{S_{m0}}{S_{00}} = \frac{S_{m0}}{q(\alpha - \alpha_0^z)}. \qquad \text{(A5)}$$

If we take into account that usually $S_{m0}\,(\alpha_0^z) \not\equiv 0$ for $m \not\equiv 0$, then a conclusion can be drawn that, α_0^z is a pole of the improper scattering matrix $\tilde{S}$. Two observations are worth mentioning:

(1) This pole of the improper scattering matrix is not a physical one and is not connected with any surface wave, contrary to the pole of the proper scattering matrix.

(2) All the zeros of the zeroth reflected order, regardless of their physical nature, are connected with poles lying on one and the same improper Riemann sheet, defined by the improper choice of the sign of χ_0.

* L. Mashev is deceased.

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