Effects of total internal reflection on the reflectivities of dielectric gratings

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We point out that the phenomenon of total internal reflection appearing on interaction of an electromagnetic wave, incident from a dielectric at the corrugated interface separating this medium from vacuum, can give rise to very large reflectivities (close to 100%), even at angles of incidence with the mean plane of the interface that are well below the critical angle. Computer simulations for sinusoidal corrugations show >90% efficiency in the zeroth reflected order for an appropriate choice of the grating period and amplitude and of the wavelength of the incident wave at normal incidence. Blaze effects, analogous to those taking place in metallic gratings, also appear. An analysis of this phenomenon in terms of resonances created under this interaction is presented.

1. INTRODUCTION

Dielectric surface-relief gratings are of interest and have applications in, e.g., fiber and integrated optics, quantum electronics, spectroscopy, and holography.[1] These gratings operate in transmission and are able to switch the diffracted energy to a given refracted order.[2,3]

One can ask, however, whether it is possible to obtain dielectric gratings that are capable of producing a substantial diffracted intensity in the reflected orders at low angles of incidence. In this way, one might devise a system that could switch the incident energy into either a transmitted or a reflected order, on control of small changes in the wavelength or in the angle of incidence. It is to be noted that this phenomenon was previously observed for a dielectric waveguide placed in vacuum.[4]

In this paper we demonstrate that this is indeed possible for a dielectric grating if total internal reflection takes place because of the corrugation of the gratings. As a matter of fact, it has been shown[5] that a randomly rough interface, separating a semi-infinite dielectric from a vacuum, can produce a remarkable reflectance when the light is incident from the denser medium, even at angles of incidence much lower than the critical angle with respect to the mean plane (as a result, such a random interface is able to yield enhanced backscattering,[6] in contrast with what happens when the light is incident from the rarer medium). Therefore, it seems natural to inquire whether periodically corrugated interfaces can produce high reflectivities under the same conditions.

2. NUMERICAL OBSERVATIONS: NORMAL INCIDENCE

The diffraction geometry under consideration is depicted in Fig. 1, namely, a linearly polarized plane wave of wavelength λ is incident at an angle θ_0 upon a sinusoidal interface of period d and amplitude $h/2$. This interface separates a dielectric of permittivity $\epsilon_{\mathrm{I}} > 1$ in which the incident wave propagates from vacuum ($\epsilon_{\mathrm{II}} = 1$).

By using a numerical code that was previously developed,[7] we have conducted calculations for $\epsilon_{\mathrm{I}} = 4$, $\epsilon_{\mathrm{II}} = 1$, $h = 0.6$, $d = 1$, and $\theta = 0°$. The wavelength of the incident wave (in vacuum) λ_0 is varied from $\lambda_0 = 0.2$ to $\lambda_0 = 2$, namely, the wavelength in the dielectric medium varies from $\lambda = 0.1$, where $\lambda = \lambda_0/n$, $n = \epsilon_{\mathrm{I}}^{1/2}$, and d, h, and λ_0 are given in arbitrary units. In these conditions the reflectivity of the perfectly plane interface is equal to 11.1%.

Figure 2 shows the efficiency of the zeroth reflected order for s (TE) and p (TM) polarization versus λ_0. As can be seen, for $\lambda_0 = 1.02$ one obtains $I_0^s = 0.98$ and $I_0^p = 0.53$. In other words, the efficiency of the zeroth reflected order is almost 100%. Also, there are other values of λ_0 for which this grating can yield >70% of the diffracted energy in the zeroth reflected order and also for p polarization. It is also interesting that the maxima of the efficiency often appear close to the Rayleigh wavelengths, and in many instances this anomaly produces a sudden drop in the value.

Phenomena of enhanced reflectivity analogous to that shown in Fig. 2 have been obtained for other combinations of parameters d, h, and λ_0, although they are not shown here for the sake of brevity. We just point out that, for example, for $\lambda_0 = 1.026$, $d = 1$, and $h = 0.8$ one obtains $I_0^s = 0.77$ and $I_0^p = 0.87$. As another example, for $\lambda_0 = 1.06$, $d = 1$, and $h = 0.7$ the result is $I_0^s = 0.41$ and $I_0^p = 0.83$.

It is worth stating that we never obtained high efficiencies for values of λ_0 larger than those shown in Fig. 2. This implies that, for $\lambda_0 > 2$, which is the case for which the grating produces only one reflected propagating order,

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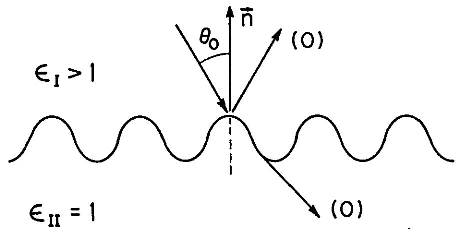

Fig. 1. Diffraction geometry.

we never observe a large reflected efficiency at low angles of incidence, regardless of the values of d and h. We believe that this fact is connected with an effect that was previously observed both in grating and rough surface theory[8,9] according to which the interface tends to behave like a flat surface as the lateral size of the corrugation tends to zero below the wavelength value.

Other profiles have been studied. For example, the triangular grating with apex angle smaller than 120° can yield high efficiency in the zeroth reflected order at normal incidence, e.g., $I_0^s = 0.53$ and $I_0^p = 0.72$ at $\lambda_0 = 1.04$. Note that in this case the local angle of incidence of the incident wave vector with the local outward normal of the interface remains larger than 30°, which is the critical angle for $\epsilon_I = 4$ and $\epsilon_{II} = 1$. On the other hand, the lamellar grating behaves almost as a flat interface, e.g., $I_0^s \approx I_0^p \approx 0.11$ at $\lambda_0 = 1.04$.

It should also be noted that for smaller values of ϵ_I one does not obtain such large efficiencies in reflection. On the other hand, the dielectric grating depicted in Fig. 3, which consists of a layer of permittivity $\epsilon_{II} > 1$ between two media of permittivities $\epsilon_I = \epsilon_{III} = 1$ (vacuum), with a periodically modulated face and thickness L, yields just one reflected order with high efficiency (the zeroth order). For example, for the parameters for which we obtained maximum efficiency in Fig. 2, namely, $\lambda_0 = 1.02$, $d = 1$, and $h = 0.6$, there exists only one reflected order in the medium with ϵ_I at normal incidence, and for $L = 4$, yielding $I_0^s = 0.98$ [the orders (1) and (−1), reflected by the corrugated side, propagate in the layer].

3. OTHER ANGLES OF INCIDENCE: BLAZE EFFECTS

Large efficiency of a dielectric grating in the antispecular direction that is due to total internal reflection can occur not only at normal incidence as shown in Section 2, but like metallic gratings (see Refs. 1 and 10) they can produce blaze in the antispecular direction when they are operated in a Littrow mounting at other angles of incidence, namely, at angles θ_0 in which the Bragg condition holds:

$$2d \sin \theta_0 = n\lambda \qquad (n \text{ is an integer}). \tag{1}$$

To illustrate this, in Fig. 4 we plot the efficiencies for s polarization when $n = 0, -1, -2$, and -3 is the index of the order that becomes antispecular at those values of θ_0 at which Eq. (1) is fulfilled. The grating profile is sinusoidal, as shown in Fig. 1, with $d = 1$, $h = 0.46$, and $\lambda_0 = 0.694$; $\epsilon_I = 4$; $\epsilon_{II} = 1$. The angles of incidence at which the corresponding orders become antispecular are $\theta_0 = 0°$ ($n = 0°$); $\theta_0 = 10°$ ($n = -1$); $\theta_0 = 20.3°$ ($n = -2$); $\theta_0 = 31.36°$ ($n = -3$). As shown in Fig. 4, the efficiencies are maxima exactly at those values of θ_0 at which the orders become antispecular. This behavior, which is a consequence of the reciprocity theorem, has been previously shown and demonstrated for metallic gratings.[10,11] Also, as in metallic gratings,[10,12] the specular and antispecular orders oscillate versus h. Figure 5 shows this fact for I_0^s and I_{-1}^s with $d = 1$, $\lambda_0 = 0.694$, and $\theta_0 = 10°$.

4. EXPLANATION OF THE ENHANCED REFLECTIVITY PHENOMENON FROM SURFACE WAVES AND RESONANCE EFFECTS

The phenomena of enhanced reflectivity observed, for example, in Fig. 2 can be classified as grating anomalies. The term anomaly, employed by Wood at the beginning of the century,[13] is currently used in the study of metallic gratings. It denotes either a rapid variation of the efficiency of such a grating when one parameter (λ_0 or θ_0, for example) is slightly varied, or a strong absorption of light by the grating. For these metallic gratings, a phenomenological theory of anomalies from excitation of surface-plasmon waves or groove resonances was developed. First, this theory provided an explanation of the origin of the anomalies and presented elementary rules for predicting quantitatively the form of the efficiencies near the anomaly.[13] Moreover, it permitted the discovery of a new phenomenon: the total absorption of light by a metallic grating.[14] We are inclined to believe that a simi-

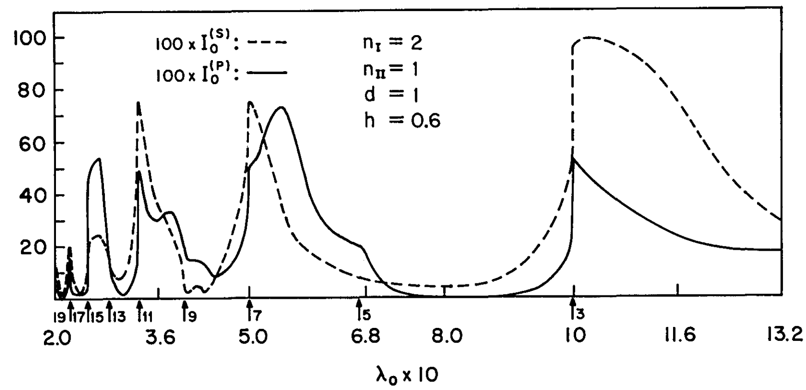

Fig. 2. Percentage efficiency in the zeroth reflected order versus the wavelength (in vacuum) λ_0 of a dielectric grating with $d = 1$ and $h = 0.6$; at normal incidence $\epsilon_I = 4$, $\epsilon_{II} = 1$. The arrows indicate the Rayleigh wavelengths. The number close to each arrow indicates the number of propagating reflected orders that exist for values of λ_0 to the right of the corresponding wavelength.

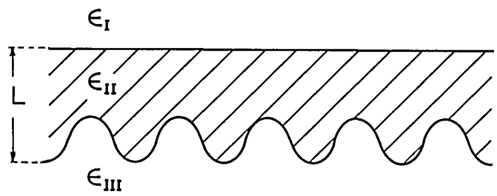

Fig. 3. Grating consisting of a slab of thickness L with the lower face corrugated.

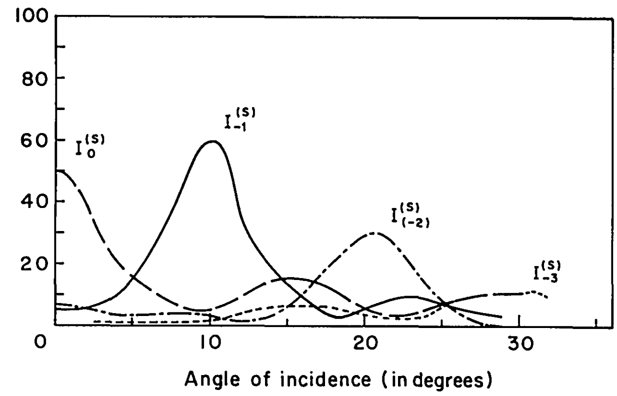

Fig. 4. Reflected efficiencies versus angle of incidence for the grating of Fig. 1 with $d = 1$, $h = 0.46$, and $\lambda_0 = 0.694$; $\epsilon_I = 4$, $\epsilon_{II} = 1$; s polarization.

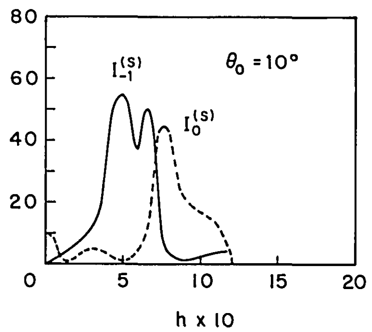

Fig. 5. Variation of the specular I_0^s and antispecular I_{-1}^s orders with h at $\theta_0 = 10°$, $d = 1$, $\lambda_0 = 0.694$.

lar explanation should be able to account for the enhanced reflectivity of dielectric gratings.

First, we give the phenomenological basis of our explanation of dielectric grating anomalies. With this aim, we consider the special grating in Fig. 6. This grating is formed by dielectric circular cavities separated by a vacuum and tied with the dielectric bulk by thin plane dielectric waveguides. Obviously, one of these cavities may have resonance frequencies. One may interpret this resonance as a consequence of the fact that a ray of light in the cavity can be reflected many times on the dielectric–vacuum circular interface. This resonant field leaks for two reasons. First, the field may be radiated in the dielectric bulk from the thin dielectric waveguide (arrow a). Second, it may be radiated on both sides (dielectric bulk or vacuum) or to an adjacent cavity by a tunneling effect through the evanescent waves (arrows b). This shows that the cavity resonance may propagate along the grating interface by successive resonant excitation of the dielectric cavities. It has been established that the existence of such a surface wave entails the existence of poles and zeros of the scattering matrix in the complex plane of λ_0. The interested reader may find the proof of this assertion, as well as a review of the phenomenological theory of metallic grating anomalies in Ref. 13. In the context of dielectric gratings, this means that, for example, the intensities I_0^s or I_0^p of the reflected zero order can be expressed by the so-called phenomenological formula as follows:

$$I_0^{s,p} \cong \left| A^{s,p} \frac{\prod_{m=1}^{M} (\lambda_0 - a_m^{s,p})}{\prod_{n=1}^{N} (\lambda_0 - b_n^{s,p})} \right|^2, \tag{2}$$

where $A^{s,p}$ is a complex multiplication factor and $a_m^{s,p}$ and $b_m^{s,p}$ are, respectively, the zeros and poles in the complex plane of λ_0. This expression takes into account the fact that, in general, more than one surface wave can propagate at the surface of the grating. In principle, each zero can be associated with a given pole and vice versa, which entails $N = M$. However, from a practical point of view, only a few number of poles and zeros play a significant role, and hence the number M of zeros to keep in the expression is not necessarily the same as the number N of poles. For example, if the zero $a_n^{s,p}$ is close to the domain of λ_0 of interest, while the associated pole $b_n^{s,p}$ is far from the domain of interest, the factor containing this pole can be considered a constant and may be omitted, its contribution being integrated into the multiplication factor $A^{s,p}$.

It is worth noting that the transmitted intensity can also be expressed in the same form as in Eq. (2) by keeping the same values of the poles $b_n^{s,p}$ (they are nothing more than the constant of propagation of the surface waves that can propagate on the grating surface) but with different zeros $a'^{s,p}_n$.

Of course, one could think that the actual gratings studied in this paper are quite different from those of Fig. 6. Nevertheless, it can be stated that one can go from the profile of Fig. 6 to a sinusoidal profile by a continuous deformation, a fact that means that the poles and zeros may be quite different but should not disappear. From an intuitive point of view, one can think that the leaks of the surface waves supported by our sinusoidal gratings are higher than the leaks of the surface waves supported by the grating of Fig. 6 since the resonant cavity of our sinusoidal grating has a larger aperture. Thus the imaginary part of the poles should be higher.

In fact, for our sinusoidal gratings, the existence of resonant excitation of surface waves and the form of the

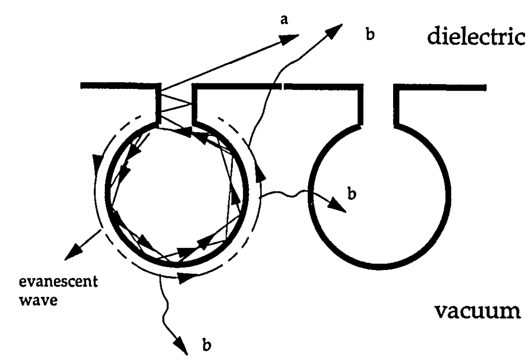

Fig. 6. Existence of surface waves on a dielectric grating explained from the propagation of a resonance of the fields in the grooves.

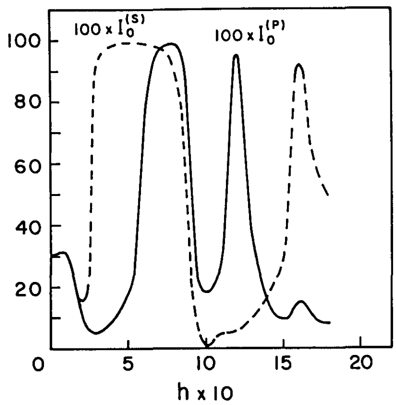

Fig. 7. Variation of the zeroth reflected order for s and p polarization versus h for the grating of Fig. 3 with $d = 1$, $\lambda_0 = 1.02$, $L = 4$; $\epsilon_{I} = \epsilon_{III} = 1$, $\epsilon_{II} = 4$.

reflected or transmitted efficiency in the zero order are confirmed by many facts. For example, if the numerical calculation of the reflected and transmitted intensities is made after a small imaginary part is introduced into the dielectric refractive index (e.g., $n = 2 + i0.01$), a strong absorption by this joule effect (more than 60%) arises, which leads us to believe that the field in the groove of the grating is quite large. Furthermore, the oscillatory behavior of the efficiencies of reflected orders (see, for example, Fig. 5) may be found as well in the transmitted efficiencies. This may lead us to the conclusion that the origin of these oscillations is the same: the resonant excitation of surface waves. For example, Fig. 7 shows the oscillations of efficiencies of the zeroth reflected order in normal incidence for both s and p polarizations for a geometry corresponding to that of Fig. 3 ($d = 1$, $\lambda_0 = 1.02$, $L = 4$; $\epsilon_{I} = \epsilon_{III} = 1$). The transmitted and reflected zeroth orders are the only nonevanescent orders, the efficiency of the zeroth transmitted order is simply $1 - I_0^{s,p}$. It is to be noted that this expression has the same poles as $I_0^{s,p}$ but different zeros, a fact that explains the different shapes of these efficiencies.

Finally, in order to prove the existence of the poles and zeros, we have used our rigorous computer codes[7] in order to find them, first using a discretization in the complex plane, then a Newton method to pinpoint the location of the poles and zeros. Figure 8 shows the trajectories in the complex plane of λ_0 of two poles and two zeros of the amplitude of the zeroth reflected order with groove depth h of a sinusoidal grating of groove spacing $d = 1$, that is illuminated in normal incidence with a p-polarized light. We are concerned here with the region defined by $0.5 < \mathrm{Re}\{\lambda_0\} < 1$.

It should be noted that the extremities of the above interval contain branch points of the amplitudes of the reflected and transmitted orders (passing off of propagating orders) and that the range of validity of the phenomenological formula obviously cannot exceed the interval between two successive branch points. It is important to note that the imaginary parts of the poles and zeros are rather large, a fact that confirms that the losses of the surface waves are important.

For $h = 0.9$ we have compared the actual efficiency of the reflected zero order, computed directly from our rigorous computer code, with the same efficiency computed by introducing the actual values of the two poles and zeros in the phenomenological formula and fitting the value of A^p. Even though a qualitative agreement appeared, a strong quantitative discrepancy remained, whatever the value of A^p. This led us to believe that the behavior of the reflected efficiency in the range of wavelengths given above was conditioned not only by the poles and zeros contained in this range, but also by poles or zeros located in the vicinity of this range. Unfortunately, cuts in the complex plane do not allow us to locate these poles and zeros. Thus, observing the discrepancy between the actual and reconstructed efficiencies by using two poles and two zeros, we conjectured that the main origin of this discrepancy was the presence of a zero around the branch point $\lambda_0 = 1$. We introduced a third zero in the phenomenological formula, the location of this third zero being roughly fitted in order to have the best agreement with the actual efficiency. Figure 9 shows the actual and reconstructed reflected efficiencies that were obtained by taking a third zero $a_3^p = 0.92 - i0.1032$. The reader may be surprised to see that this zero is contained in the range of interest since its real part is less than one. In fact, this zero does not exist, but it simulates, at best, the influence of poles and zeros located on both sides of this domain of interest as well as the influence of the branch points. The quantitative agreement on a large part of the curves is almost perfect, but significant discrepancies hold on both extremities (~25% at the top of the resonance peak). This is not surprising since the phenomenological formula is not able to take into account the branch points at the extremities of the interval. A better agreement could be obtained either

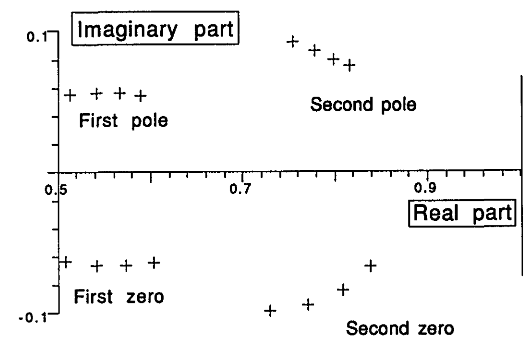

Fig. 8. Location of the poles and zeros in the complex plane of λ_0 for a dielectric sinusoidal grating of period $d = 1$ illuminated in normal incidence. For each pole or zero, the crosses represent the locations that correspond to $h = 0.8, 0.9, 1.0$, and 1.1, from left to right.

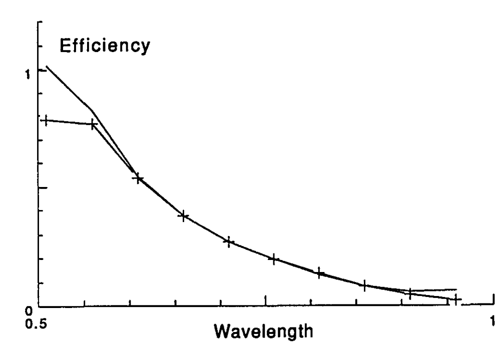

Fig. 9. Rigorous (crosses) and reconstructed reflectivity of the grating of Fig. 8 with $h = 0.9$.

by increasing the number of poles and zeros outside the region of interest or by modifying the phenomenological formula in order to introduce branch points. However, the relatively good agreement obtained in Fig. 9 shows without any doubt that the phenomenon of enhanced reflectivity for dielectric gratings is due to the presence of poles and zeros in the complex plane of λ_0. These poles and zeros are a consequence of the resonant excitation of surface waves.

5. CONCLUSION

We have shown that a modulated interface may produce a phenomenon of enhanced reflectivity near normal incidence when an incident wave propagates from a dielectric medium to the vacuum. The same phenomenon arises for nonnormal incidence near the Littrow mount.

An explanation of this phenomenon has been given in terms of excitation of surface waves that are due to the propagation of resonances in the dielectric grooves (total internal reflection). This phenomenological explanation leads to a phenomenological formula giving the reflected efficiency from a knowledge of some poles and zeros in the complex plane of the wavelength. This formula has provided the reflected efficiency with good quantitative agreement.

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