Lamellar metallic grating anomalies

E. Popov, L. Tsonev, and D. Maystre

A detailed numerical investigation of anomalies in lossy metallic lamellar gratings is presented in a large interval of a wavelength-to-period λ/d ratio. A substantial increase in absorption (a decrease in the total diffracted energy) is observed. If λ/d is small enough (within the homogenized limit), the absorption can reach almost 100%. When the groove width is large enough, the anomalies are connected with mode resonances inside the grooves.

Introduction

Since 1902 when Wood[1] made his important observation that the intensity of light diffracted by a reflection grating could vary greatly in a narrow wavelength (or angular) interval, this phenomenon, which he called anomalous, has been the subject of great scientific interest. First, avoiding anomalies is vital to increasing the performance of spectroscopic devices. Second, anomalies can lead to a significant increase in absorption. The most illustrative example is the so-called Brewster effect in shallow reflection gratings[2]; otherwise in specific conditions a highly reflecting metallic surface with a shallow corrugation can absorb incident light totally. These conditions provide excitation of a surface wave along the corrugated metal–air interface. Later[3] it was shown that similar phenomena could exist for deep metallic gratings. Today it is well known that they have a resonance nature, and consequently they are accompanied by significant field enhancement; the electromagnetic field density near the corrugation becomes 50–100 times or more greater than the corresponding energy density for a flat mirror made from the same material—a fact that is of separate interest.[4–11]

In contrast to this resonance behavior in some cases the increase in the absorption of corrugated metallic surfaces is not accompanied by noticeable field enhancement, the electromagnetic energy density exceeding the corresponding density for a flat mirror by a factor not greater than 5–10. Such absorption was observed in metallic gratings under a grazing incidence[12] and in very deep lamellar metallic gratings (depth-to-period ratio > 0.3).[13]

In 1979 Andrewartha *et al.*[14,15] studied perfectly conducting lamellar diffraction gratings in detail. They discovered that modes exist inside the grooves, their number depending on the groove width and wavelength. In certain conditions these modes can be excited, causing a strong redistribution of energy into different diffraction orders in the far-field region. The conditions in which mode resonances are transferred into resonances of the diffracted field depend on wavelength and groove depth. These resonances do not lead to absorption because, as indicated in Refs. 14 and 15, the substrate is assumed to be perfectly conducting. Much research has been done in the last decade to produce a theoretical method that could deal with lossy lamellar gratings.[16–20] Unfortunately the problems increase for highly reflecting materials, which is of predominant interest.

Recently Popov and Tsonev[13] on the basis of a rigorous modal theory[16,17] were able to establish the existence of 100% light absorption when the grating supports only a single (specular) diffracted order—the grating can absorb the incident light almost totally. Surprisingly this absorption is not accompanied by field enhancement inside or outside the grooves. The electromagnetic energy density does not exceed twice the energy density of the incident wave, whereas for a highly reflecting flat mirror this ratio almost reaches a value of 4. The aim of this paper is to investigate in greater detail light absorption by deep lamellar gratings. The current numerical study covers a considerably large d/λ region—from gratings that support several diffraction orders to the so-called homogenized case ($\lambda/d \ll 1$). In the

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entire interval the anomaly can be observed clearly, which changes its depth in the different regions. Our aim was also to throw some physical light on the nature of this anomaly and in particular to demonstrate its connection with mode resonances inside highly conducting well-separated grooves when the period is large enough.

During the preparation of this paper Glytsis and Gaylord[21] published a detailed study of high-spatial-frequency binary gratings for both TE and TM polarizations. In the long wavelength limit the behavior of these gratings becomes equivalent to a homogeneous layer. Our conclusion confirms this finding even in the anomalous region; i.e., the strong absorption in the case of $\lambda/d \ll 1$ is equivalent to the absorption of a homogeneous lossy layer with a refractive index given by the homogenization formula.[22]

We obtained the results presented here by using a computer code based on the rigorous modal method for lossy lamellar gratings.[16] The eigenvalues of the modal equation were found by use of two independent schemes,[16,17] which were checked against each other. The rigorous integral formalism[23] was used to test the results of the modal method, and no significant discrepancy was noticed even inside the anomalous regions.

Light Diffraction by Lamellar Metallic Gratings

TE-polarized light (with the electric-field vector parallel to the grooves) with a wavelength of $\lambda = 1$ μm is incident normally (angle of incidence $\theta = 0$) from the vacuum on a metallic lamellar grating with a groove depth of $h = 1$ μm. All the notations and the coordinate system are presented in Fig. 1. The complex refractive index of the lamella and the substrate material is equal to $n_s = 0.4 + i4.4$. We worked at a fixed wavelength, varying the grating period d to eliminate the influence of the refractive-index dispersion. Under normal incidence the number of diffraction orders propagating in the cladding depends on the period-to-wavelength ratio: one for $d/\lambda < 1$, three for $1 < d/\lambda < 2$, five for $2 < d/\lambda < 3$, etc. When the lamella width w is varied, the redistribution of energy into different propagating orders ($d/\lambda > 1$) is observed even for a perfectly conducting case, but the sum of their efficiencies remains equal to unity. For real metallic gratings there are always losses caused by the absorption. The sum of efficiencies of the propagating diffraction orders (i.e., the total energy diffracted in the cladding, normalized with respect to the energy of the incident wave) is potted in Fig. 2 as a function of grating period and lamella width. On the high background level (where reflectivity of the corresponding flat mirror exceeds 92%) several dips can be observed. Their depths decrease with an increase in the period. Three regions can be distinguished clearly:

(1) $d/\lambda < 0.3$. The dip in the reflectivity is well defined with a minimum value of less than 10%. Its location in the $(d) - (w/d)$ plane is almost independent of d. This case corresponds to the so-called homogenization limit and is referred to below as the homogenized case.

(2) $d/\lambda > 0.8$. The reflectivity dips lie on hyper-

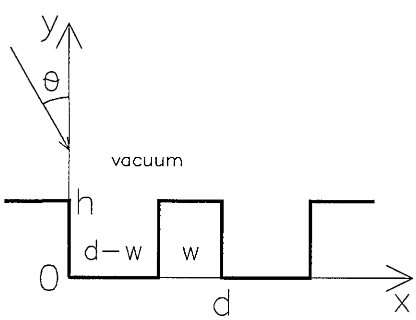

Fig. 1. Schematic representation of a lamellar grating.

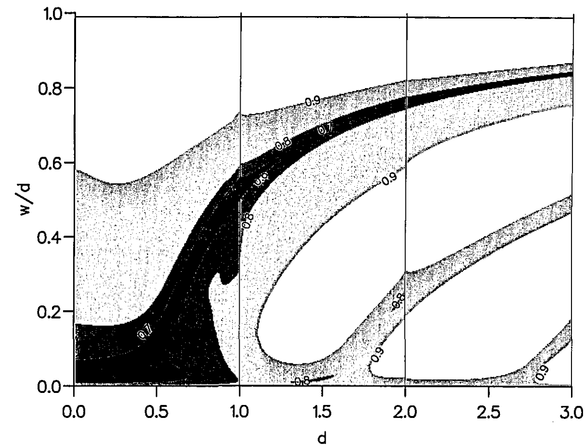

Fig. 2. Total energy diffracted by the grating (the sum of diffracted order efficiencies) as a function of period d (given in micrometers) and the filling factor w/d (w is the lamella thickness). Groove depth $h = 1$ μm, wavelength $\lambda = 1$ μm. The TE-polarized light has normal incidence on a metallic grating with a refractive index equal to $0.4 + i4.4$.

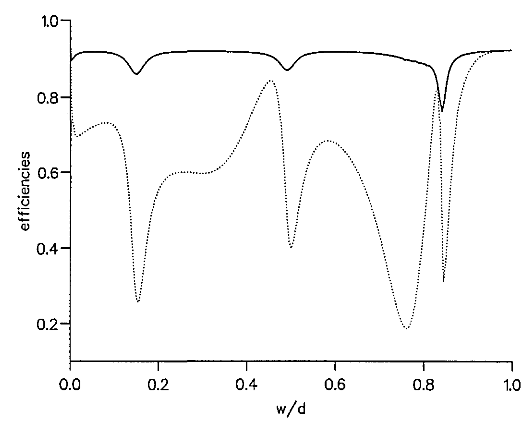

Fig. 3. Total reflected energy (solid curve) normalized with respect to the incident wave energy and the zeroth-order efficiency (dotted curve) as a function of filling factor w/d for fixed period $d = 2.99$ μm. The other parameters are the same as those in Fig. 2.

bolas described by

$$w/d = 1 - c_i/d, \tag{1}$$

where c is a constant that determines the position of the minima in the $(d) - (w/d)$ plane. We introduce its index i to distinguish between different minima. Contrary to the homogenized case this case is referred to below as the grating case. Although these notations are rather arbitrary, they correspond to the real physical situation.

(3) The intermediate case, in which the two regions merge with each other and the behavior of the anomaly cannot be defined simply.

Grating Case

The total energy E_t diffracted by the grating is almost independent of the grating parameters, except for relatively small regions. Although the groove depth is comparable with the period, E_t outside these anomalous regions is almost equal to the reflectivity of a flat surface. When the grating supports several orders their efficiencies exhibit more complicated behavior

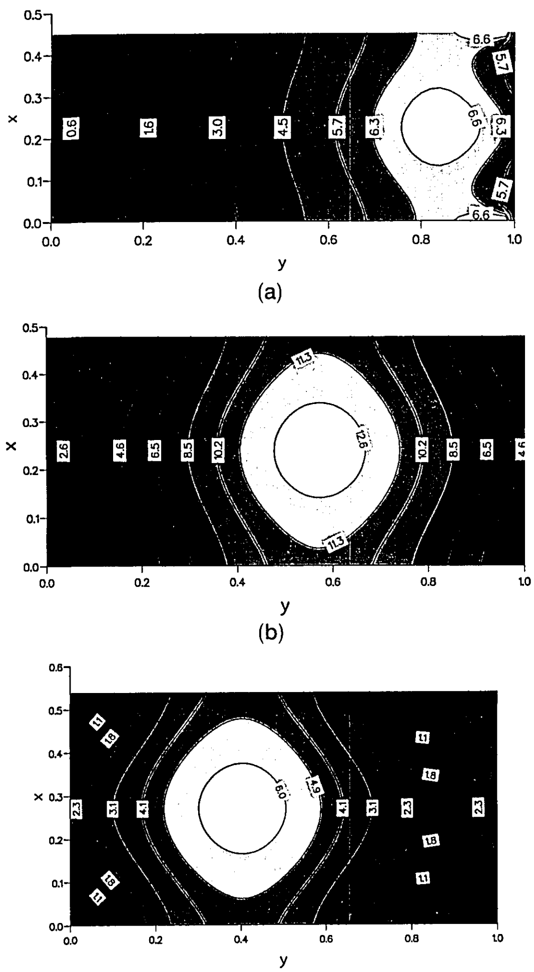

Fig. 4. Maps of the electromagnetic energy density inside the groove, which corresponds to Fig. 2: (a) $w/d = 0.85$; (b) $w/d = 0.84$, (c) $w/d = 0.82$. Units of the x and y axes are in micrometers. Period $d = 2.99$ μm.

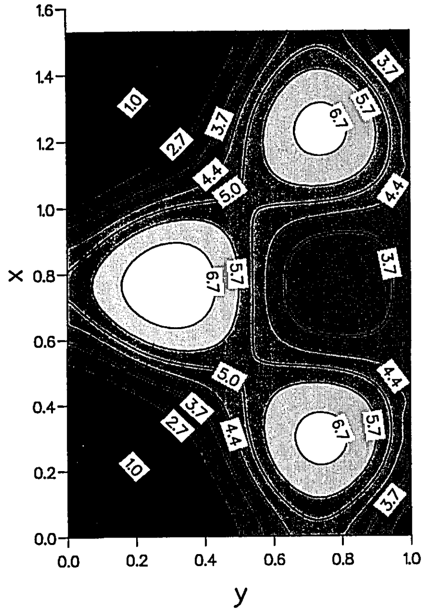

Fig. 5. Same as Fig. 4 except that $w/d = 0.49$.

(Fig. 3), which is our main reason for dealing with E_t rather than with a particular order of efficiency.

The position of the minima is described by Eq. (1), which is equivalent to

$$d - w = c_i, \tag{2}$$

where $d - w$ is the groove width (w is the lamella width). Therefore the anomalies are exhibited at some fixed values c_i of the groove width, which do not depend on the period and on the lamella thickness. This fact points to a direct link between the position of the anomaly and the behavior of the electromagnetic field inside the groove. Figure 2 presents a picture that resembles modal dispersion characteris-

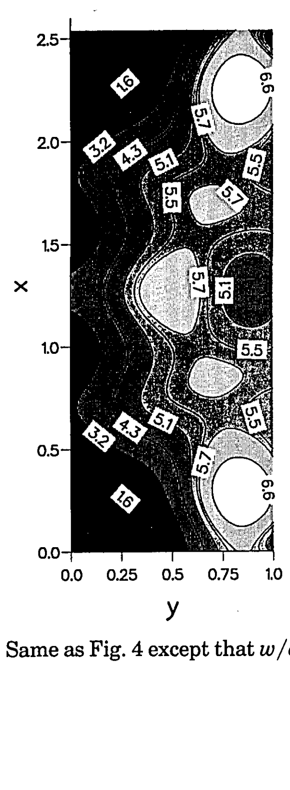

Fig. 6. Same as Fig. 4 except that $w/d = 0.15$.

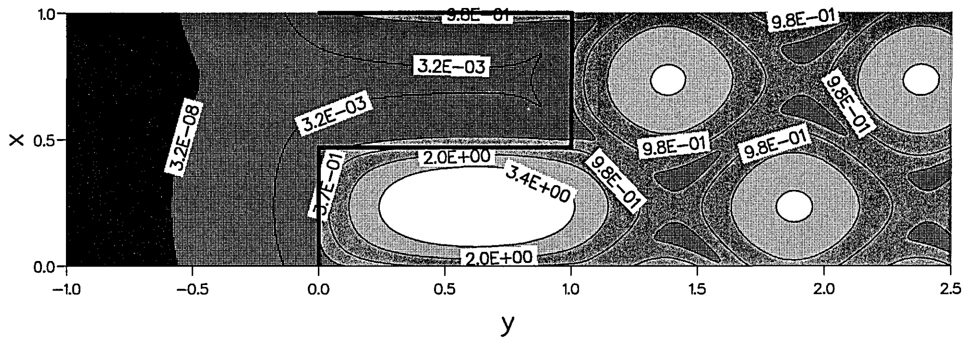

Fig. 7. Map of the TE-field component E_z for $d = 1$ μm and $w/d = 0.53$. The heavy solid line represents the groove profile.

tics. It is well known from the early research of Andrewartha *et al.*[14,15] that for a perfectly conducting lamellar grating the groove mode resonances do not depend separately on the groove period or lamella thickness but on the groove width, because the perfect conductivity prevents the coupling of the field in the neighboring grooves directly through the lamella walls. As mentioned above, for perfectly conducting gratings no dips in the total reflectivity are observed in contrast with the lossy case in Figs. 2 and 3.

All these considerations provide a natural reason to examine the field distribution inside the grooves in the anomalous regions. In Figs. 4–6 a two-dimensional cross-sectional map of electromagnetic energy density, normalized with respect to the incident energy, is presented for different values of the groove width $d - w$, which illustrates from the microscopic point of view the three peculiarities of the reflectivity curve of Fig. 3. The figures are ordered in the direction of increasing groove width. The field distributions in Fig. 4 correspond to the first (deepest) anomaly around $w/d = 0.84$, i.e., at the smallest groove width $(d - w)/d = 0.16$. A well-distinguished maximum of the lowest groove mode can be observed. Its evolution with an increasing groove width can be followed easily, whereas for $(d - w)/d = 0.15$ the groove is a little narrower for the mode, and at $(d - w)/d = 0.18$ a formation of the second mode has already started; the intermediate width $(d - w)/d = 0.16$ is most suitable for fitting the mode inside the groove. Not surprisingly, the 0.16 value corresponds to the position of the first dip in the reflectivity. As expected, the second and third dips appear when the groove becomes wide enough for higher modes to exist (Figs. 5 and 6). At normal incidence the symmetry of the system forbids excitation of antisymmetrical modes (with an even number of maxima), and only those with an odd number of maxima lead to an anomaly in the reflectivity [Figs. 4(b), 5, and 6].

Strictly speaking, mode resonances are described mathematically by poles of the scattering matrix, whereas the zeros of the propagating order amplitudes play the major role in the formation of dips in the efficiency curves. When the media are lossy and in cases of multiple propagating orders, these poles and zeros are complex with high imaginary parts, and their influence on the reflectivity behavior is very complicated. Instead of analyzing their behavior, we tried to draw a connection between anomalies in the reflectivity and the field density distribution, which has a more direct physical meaning, although this connection is more difficult to describe mathematically.

The finite conductivity of the lamellae causes the transverse component of the electromagnetic field on the surface to differ from zero, leading to absorption losses. As a result of the field penetration in the metal, there is direct coupling between the modes in the neighboring grooves. The coupling is negligible for lamellae with higher optical thicknesses, which is why the anomalies follow phenomenological rule (1) well in a very large domain. Even for values of $d = 1$ μm and $w/d = 0.53$ when the reflectivity is less than 32%, the direct coupling of the field through the lamellae is very weak (Fig. 7). The coupling becomes important for very thin lamellae [in the region of $(d - w)/\lambda \ll 1$ in Figs. 2 and 3]. Note that in this region the total diffracted energy can become considerably low. The position and the values of the minima depend strongly on the groove depth. A detailed study of the grating behavior in this intermediate region is carried out in Ref. 13, and it is shown

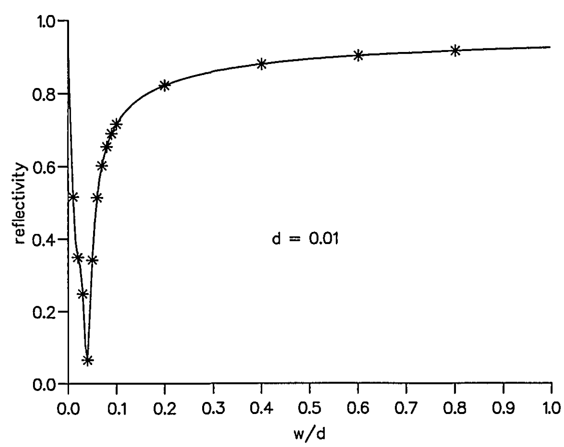

Fig. 8. Reflectivity as a function of the filling factor w/d for $d = 0.01$ μm. Solid curve, modal theory results; asterisks, reflectivity of a layer with a refractive index given by the homogenization formula [Eq. (3)].

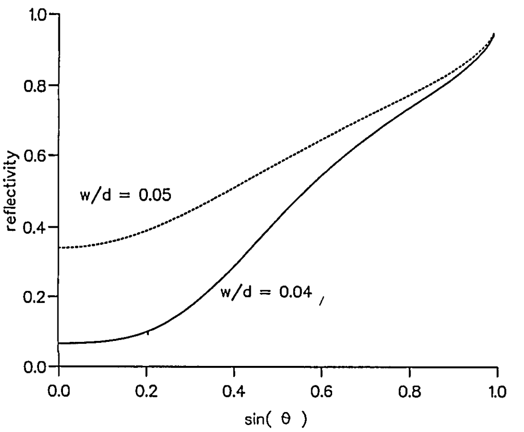

Fig. 9. Angular dependence of reflectivity for the grating discussed in Fig. 8 for two consecutive lamella width values, as indicated in the figure.

that for $h > 2$ μm the absorption could reach almost 100%. Although the maximum absorption corresponds to the mode excitation inside the grooves (i.e., a resonance process), it is not accompanied by any noticeable field enhancement near the grating surface (or in the far-field region). Strictly speaking, there are poles of the scattering matrix corresponding to the groove mode excitation, but they are located so far from the real axis that their influence is negligible for real angles of incidence.

Homogenized Case

After a further reduction in the period, we reach the well-known situation known as the homogenization of the grating. At less than some limiting value of d the incident light no longer sees the grating as a corrugated structure. The grooves and the lamellae have average influence, and the grating behaves as a homogeneous layer with average optical characteristics, isotropic in the TE case and anisotropic in the TM case.[22] Below this limit no further reduction in the period has any influence on the system response. This limiting (homogenization) value of d/λ could not be determined by theoretical considerations, and in our case the saturation value is considerably high. When $d/\lambda < 0.2$, neither the reflectivity value nor the anomaly position varies with a decrease in the period.

The average optical index n of the homogenized grating is given by[22]

$$n^2 = n_1{}^2(d - w)/d + n_2{}^2 w/d, \tag{3}$$

where n_1 and n_2 are the refractive indices of the cladding and the lamellae. The system reflectivity obtained by the rigorous modal method and by use of Eq. (3) is presented in Fig. 8. Because of the imaginary part of n_2, the layer could have high absorption. In particular, for $w/d = 0.04$ (a value corresponding to the dip in Fig. 8) the refractive index n is $0.4637 + i0.1518$. The reflectivity of such a layer deposited on a metallic substrate has a minimum of 0.057 at a thickness of $h = 0.94$ μm.

The nonresonant behavior of this anomaly results in a relatively flat angular dependence of the reflectivity (Fig. 9). This fact could be of a great practical interest, for example, in reducing the radar signal response from an object covered by such a grating.

Conclusion

A detailed numerical study of anomalous light absorption by deep metallic lamellar diffraction gratings in the large interval of groove period values has enabled us to establish important connections between this effect and mode excitation inside the grooves, when the grooves are wide enough and the lamellae are enough to provide a significant separation between the electromagnetic field inside each groove. In the case of small periods (hence a small lamella thickness as well), when the direct coupling of the field in the neighboring grooves becomes so large that the grating is homogenized, a sharp increase in absorption can be observed in a wide angular interval.

This research was done while E. Popov held a postdoctoral position in the Laboratory of Electromagnetic Optics, Marseille, France.

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