Resonant effects in periodic gratings comprising a finite number of grooves in each period

Angela N. Fantino, Susana I. Grosz, and Diana C. Skigin*

Grupo de Electromagnetismo Aplicado, Departamento de Física, Facultad de Ciencias Exactas y Naturales,

Universidad de Buenos Aires, Ciudad Universitaria, Pabellón I, 1428 Buenos Aires, Argentina

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We give numerical evidence of a kind of resonance that appears in infinite perfectly conducting gratings comprising a finite number of grooves in each period when illuminated by a normally incident *p*-polarized plane wave. This phenomenon is intimately connected with the particular distribution of the phase of the electromagnetic field inside the cavities, which is automatically generated by waves of certain resonant wavelengths. The resonances appear as sharp peaks in the specularly reflected efficiency and are accompanied by a significant intensification of the interior field. We study the particular case of rectangular cavities and consider configurations with different numbers of grooves per period. The diffraction problem is solved for *s* and *p* polarization by using the modal method, which proves to be especially suitable for this profile.

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I. INTRODUCTION

The scattering from structures comprising a finite number of elements has been recently studied in connection with the superdirective property [1-6]. In these references the authors consider different structures formed by an array of passive elements such as slotted cylinders [5] or rectangular cavities [6], to be used as superdirective antennas. The occurrence of superdirectivity can be attributed to the excitation of modes inducing a phase reversal in the adjacent scatterers. It has been found that, when the structure is illuminated by *p*-polarized waves (magnetic field perpendicular to the plane of incidence) of certain resonant frequencies, there is a very high level of stored electromagnetic energy in the interior of the array elements [5,6]. This enhancement is associated with the excitation of high-Q resonances in the system [2], and is accompanied by a particular distribution of the phase of the field in the structure. In such a case, the phase difference between adjacent cavities is 0 or π rad.

It is well known that the efficiency reflected by infinite periodic gratings can exhibit anomalies of a different nature. When a metallic grating is illuminated by *p*-polarized light, a surface plasmon polariton can be excited along the surface [7,8]. This excitation is accompanied by a significant power absorption [9,10], and consequently it produces a sudden change in the efficiency curves of the reflected orders. This phenomenon is particularly important when the corrugations are shallow. Rayleigh anomalies, caused by the appearance or disappearance of a diffracted order, are also present in infinite gratings and produce sudden variations in the efficiency response of the grating [9]. The efficiency curves of periodic gratings can also be significantly modified by the surface shape resonances that occur when the corrugations are deep, particularly if the cavities are multivalued. Under certain conditions, the eigenmodes of the cavities are excited, and this generates interesting resonant effects such as field enhancement inside the corrugations. Unlike the surface plasmon excitations, these resonances are associated with the

particular shape of each groove and can be excited by *s*-polarized light (electric field perpendicular to the plane of incidence) [11-16].

In this paper we investigate a kind of resonance that appears in infinite gratings comprising a finite number of grooves in each period (compound gratings). In particular, we consider cavities of rectangular shape. This profile allows us to investigate the influence of the different geometrical parameters of the grating (width and depth of the grooves, distance between them, and period) on the reflection response, particularly on the resonant phenomenon. In addition, since this shape is easy to manufacture, we believe that experiments confirming these resonances could be performed.

The formalism used to solve the problem of diffraction from an infinite periodic grating with several grooves in each period is an extension of that presented by Andrewartha *et al.* for a perfectly conducting grating with rectangular grooves [11]. This is a rather simple and efficient method that also allows us to understand the resonant character of the grating in terms of the eigenmodes of the grooves, which are known to play an important role in the generation of this phenomenon.

The purpose of this paper is to address numerical evidence of the resonant phenomenon that takes place in infinite gratings comprising a finite number of grooves in each period. These resonances are intimately connected with the particular distribution of the electromagnetic field inside the corrugations, and appear as sharp peaks in the specular reflectance of the grating. Therefore, this phenomenon could be used in devices involving selective processes such as filters and polarizers.

This paper is organized as follows. In Sec. II we outline the modal method applied to a perfectly conducting grating with several rectangular grooves in each period. To study the influence of the number of grooves on the resonant response, we give and discuss the numerical results obtained for gratings comprising one to seven grooves per period. We consider gratings comprising up to 19 grooves per period in order to analyze the effect of the occupancy rate between the corrugation and the planar zone. We show curves of the

^{*}Electronic address: dcs@df.uba.ar



FIG. 1. Configuration of the problem.

specular efficiency and of the amplitude and phase of the field inside the cavities as a function of the spatial frequency. We also show the magnetic field distribution in the near region for certain significant wavelengths. These results are given in Sec. III. Finally, concluding remarks are given in Sec. IV.

II. THEORY

A. Modal approach

We consider the problem of diffraction by a perfectly conducting one-dimensional grating illuminated by a monochromatic plane wave of frequency ω . Each period of the grating consists of *N* equally spaced rectangular grooves and a planar zone, as shown in Fig. 1. The structure and the fields are invariant in the *z* direction; thus the problem is reduced to a two-dimensional one. All the *N* grooves have width *a* and height *h*, and are separated by a distance *b*. The period of the grating is *d*.

We consider the two fundamental modes of linear polarization: *s* (electric field parallel to the *z* direction) and *p* (magnetic field parallel to the *z* direction). Assuming an $\exp(-j\omega t)$ time dependence for both electric and magnetic fields, and using the Maxwell equations, it is possible to represent the fields by a scalar function *f* that must satisfy the differential equation [17]

$$[\nabla^2 + k^2]f(x, y) = 0, (1)$$

where $k = \omega/c$ and c is the speed of light in vacuum. f represents the z component of the electric field (E_z) in the s-polarization case, and the z component of the magnetic field (H_z) in the p-polarization case. The x and y components of the fields can be obtained from f [17].

To solve the problem we consider three regions (see Fig. 1): in region 1 ($y \ge 0$) there is vacuum; region 2 ($-h \le y \le 0$) is the modulated zone; and region 3 ($y \le -h$) corresponds to the perfect conductor, where the fields are null. We denote the function f in the region j as f_j .

Region 1. The function f_1 is a solution of the differential equation (1) and must satisfy the radiation condition and the property of pseudoperiodicity of the fields. It can be expressed as the sum of the incident and the diffracted fields [18]:



FIG. 2. Specular efficiency versus kh for a grating with a/h = 0.3 and d/h = 6, for both cases of polarization: (a) N = 1 (simple grating); (b) N = 3 (compound grating with three grooves in the period and b/h = 0.2).

$$f_1(x,y) = e^{j(\alpha_0 x - \beta_0 y)} + \sum_{n = -\infty}^{\infty} R_n e^{j(\alpha_n x + \beta_n y)}, \qquad (2)$$

where

$$\alpha_0 = k \sin \theta_0, \tag{3}$$

$$\beta_0 = k \cos \theta_0, \tag{4}$$

$$\alpha_n = \alpha_0 + \frac{2\pi n}{d},\tag{5}$$

$$\beta_n = \sqrt{k^2 - \alpha_n^2},\tag{6}$$

 θ_0 is the incidence angle, and R_n is the unknown Rayleigh amplitude of the diffracted order *n*.

Region 2. In this region the fields must be null inside the perfect conductor, whereas inside the grooves f_2 must satisfy the differential equation (1) and the corresponding boundary conditions on the walls of each groove. Since the boundary



FIG. 3. (a) Relative amplitude of the fundamental mode versus kh; (b) phase difference between the fundamental modes of adjacent grooves. The parameters of the grating are N=3, a/h=0.3, b/h=0.2, and d/h=6, and *p*-polarized illumination.

conditions do not couple the variables x, y, it is possible to express the function f_2 in the *n*th groove $[f_{2n}(x,y)]$ by its modal expansion:

$$f_{2n}(x,y) = \sum_{m} C^{q}_{nm} g^{q}_{nm}(x) h^{q}_{m}(y),$$

$$q = s, p$$
 for s or p polarization, respectively, (7)

where

$$g_{nm}^{q}(x) = \begin{cases} \cos\{(m\pi/a)[x-(n-1)(a+b)]\}, & q=p\\ \sin\{(m\pi/a)[x-(n-1)(a+b)]\}, & q=s, \end{cases}$$
(8)

 $\mu_m = \sqrt{k^2 - (m\pi/a)^2}.$

$$h_{m}^{q}(y) = \begin{cases} \cos[\mu_{m}(y+h)], & q=p\\ \sin[\mu_{m}(y+h)], & q=s, \end{cases}$$
(9)

and

(a)



FIG. 4. Relative magnetic field intensity distribution for the same grating as in Fig. 3 and *p* polarization: (a) resonant wavelength (kh = 1.355); (b) nonresonant wavelength ($kh \approx 1.2$).

Then

$$f_2(x,y) = \sum_{n=1}^{N} f_{2n}(x,y) \operatorname{rect}\{[x - (n-1)(a+b)]/a\}.$$
(11)

Owing to the pseudoperiodicity of the fields, the boundary conditions at y=0 can be imposed in a single period only. The tangential component of the electric field must be continuous in the whole period $(0 \le x \le d)$ and the tangential component of the magnetic field must be continuous only in the interval $n(a+b) \le x \le n(a+b)+a$, $n=1,2,\ldots,N-1$. Thus we obtain a system of two equations for each polarization, where the unknowns are the Rayleigh coefficients (R_n) and the modal amplitudes (C_{nm}^q) . By projecting these equations in appropriate bases, we obtain the following equations for *s* polarization:

$$R_{l}^{s}d = -\delta_{0l}d + \sum_{m=1}^{\infty} \sum_{n=1}^{N} C_{nm}^{s} \sin(\mu_{m}h)$$
$$\times \exp[-j\alpha_{l}(a+b)(n-1)]J_{ml}^{*}, \qquad (12)$$

$$\frac{a}{2}C_{nm}^{s}\mu_{m}\cos(\mu_{m}h) = j\sum_{t=-\infty}^{\infty}\beta_{t}\exp[j\alpha_{t}(a+b) \times (n-1)]J_{mt}(R_{t}^{s}-\delta_{t0}), \quad (13)$$

(10) where

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FIG. 5. Specular efficiency versus kh for a grating with a/h=0.3, b/h=0.2, and d/h=6, for p polarization: (a) N=4; (b) N=5; (c) N=6; (d) N=7.

$$J_{ml} = \begin{cases} -(m\pi/a)[(-1)^{m}e^{j\alpha_{l}a} - 1]/[(m\pi/a)^{2} - \alpha_{l}^{2}] \\ \text{if } (m\pi/a)^{2} \neq \alpha_{l}^{2} \\ \pm a/(2j) \quad \text{if } \pm m\pi/a = \alpha_{l}. \end{cases}$$
(14)

For p polarization we get

$$\beta_{l}R_{l}^{p}d = \beta_{l}\delta_{0l}d + \sum_{m=0}^{\infty}\sum_{n=1}^{N}j\mu_{m}C_{nm}^{p}\sin(\mu_{m}h) \\ \times \exp[-j\alpha_{l}(a+b)(n-1)]I_{ml}^{*}, \qquad (15)$$

$$\frac{a}{2}(1+\delta_{m0})C_{nm}^{p}\cos(\mu_{m}h) = \sum_{t=-\infty}^{\infty}\exp[j\alpha_{t}(a+b) \times (n-1)]I_{mt}(R_{t}^{p}+\delta_{t0}),$$
(16)

$$I_{ml} = \begin{cases} j \alpha_l [(-1)^m e^{j \alpha_l a} - 1] / [(m \pi/a)^2 - \alpha_l^2] \\ \text{if } (m \pi/a)^2 \neq \alpha_l^2 \\ a/2 \quad \text{if } (m \pi/a)^2 = \alpha_l^2 \neq 0 \\ a \quad \text{if } (m \pi/a)^2 = \alpha_l^2 = 0. \end{cases}$$
(17)

By solving the system of equations (12) and (13) for *s* polarization, and the system of equations (15) and (16) for *p* polarization, we find the unknown Rayleigh coefficients (R_n^q) or the modal amplitudes C_{nm}^q .

B. Numerical considerations

The formalism presented above was implemented numerically as a FORTRAN program. The series were truncated to satisfy the matching conditions at y=0. We used 61 terms in the Rayleigh expansion to guarantee the fulfillment of these conditions, and 10 terms in the modal series were enough in all cases presented here.

where



FIG. 6. Relative magnetic field intensity distribution inside and outside the cavities, for the same gratings as in Fig. 5 and p polarization, for the π resonance: (a) N=4; (b) N=5; (c) N=6; (d) N=7.

The matrix inversion is performed by standard numerical techniques. The inversion process was also under control so that the error was always less than 10^{-11} . The control coefficients are defined as

$$c_1 = \sum_{mn} (AA^{-1})_{mn} - I_{mn}, \qquad (18)$$

$$c_2 = \sum_{mn} (A^{-1}A)_{mn} - I_{mn}, \qquad (19)$$

where A is the matrix inverted to solve the problem and I is the identity matrix.

In the *s* case, we can freely choose whether to solve the problem for the Rayleigh coefficients R_l^s (in which case the matrix has dimension $L \times L$, where *L* is the number of terms retained in the Rayleigh expansion) or for the modal amplitudes C_{nm}^s [in which case the dimension of the matrix is $(NM) \times (NM)$, where *M* is the number of terms retained in the modal series]. In the *p* case, the modal series includes the term m=0. Since $\mu_0=k$ and the zone of the spectrum we want to focus on includes the value of $kh=\pi/2$, we have $\cos \mu_0 h=0$ for a certain wavelength. Therefore, we substitute Eq. (15) in Eq. (16), and obtain a matrix equation of dimension $[N(M+1)] \times [N(M+1)]$ for the unknown modal amplitudes C_{nm}^p .

We also verified that in all cases the sum of the diffracted efficiencies is 1, within an error of 10^{-14} .

III. NUMERICAL RESULTS

In this section we present some of the results obtained for gratings with different numbers of grooves per period when the grating is normally illuminated by a plane wave. In Fig. 2(a) we show the specular efficiency as a function of kh for a simple grating (N=1) with a/h=0.3 and d/h=6, for both polarization cases. The range of λ used in all the examples was specifically chosen so that there were only three propagating orders, i.e., $\lambda/d \in [0.5,1]$. This interval includes the value of λ that makes $kh = \pi/2$, in the vicinity of which we expect the resonance for compound gratings, and it excludes any other anomalies caused by the appearance or disappearance of a propagating order. As can be observed, simple gratings do not present resonances associated with phase differences of 0 or π between adjacent grooves for either s or p polarization. This behavior was expected since each period has a single groove and, consequently, every groove is equivalent to its neighbor, and so is the interior electromagnetic field. This fact establishes that the phases of the interior field must be equal in all grooves. Due to the symmetry imposed by the normal incidence, the same argument can be applied to a grating with two grooves per period. This fact has been numerically verified.

However, in gratings comprising three or more grooves per period, a resonant phenomenon like that described in [6] for finite structures is expected. In this paper we demonstrate this effect numerically and illustrate the resonant phenomenon in infinite gratings in the following figures. In Fig. 2(b) we plot the efficiency curve for a grating formed by three



FIG. 7. (a) Relative amplitude of the fundamental mode versus kh for a grating with N=5; (b) same as (a) for N=6; (c) phase difference between the fundamental modes of adjacent grooves, for the same configuration as in (a); (d) same as (c) for N=6. The other parameters of the grating are: a/h=0.3, b/h=0.2, and d/h=6, and p-polarized illumination.

rectangular equally spaced grooves with a/h=0.3, b/h = 0.2, and d/h=6. Note that in this case the corrugated zone occupies 25% of the period. It can be observed that there is a peak in the case of *p* polarization, whereas no peak is present in the *s* case.

As explained in Sec. II, the interior field is expressed in terms of the eigenmodes of the cavities. In the examples studied here, we found that the amplitude of the fundamental mode is at least 10^6 times greater than the other amplitudes. Therefore, in a first approximation, we can evaluate the behavior of the field inside the cavities by considering the fundamental mode only. In Fig. 3 we plot the fundamental amplitude of each cavity relative to the amplitude of the incident plane wave [Fig. 3(a)] and the phase difference between the fundamental modes of adjacent grooves [Fig. 3(b)] vs kh, for the same structure considered in Fig. 2. Owing to the symmetry imposed by the normal incidence, we expected the fields in the extreme grooves to be equal. This can be observed in Fig. 3. It should be noted that when the phase difference is $\pm \pi$ the specular efficiency has a maximum [Fig. 2(b)]. In the inset in Fig. 3(b) we schematized the resonant configuration as follows. The first groove was arbitrarily assigned a plus sign. Then we consider the phase difference between one groove and the preceding one. If the difference is 0, the sign will be the same as that of the preceding one. But if the difference is π the groove will have the opposite sign. This procedure is repeated for each groove. For instance, the resonant configuration is [+-+] for three grooves.

In Fig. 4 we show contour plots of the magnetic field relative to the incident field in the vicinity of the structure. Figure 4(a) corresponds to the resonant wavelength (kh = 1.355) whereas Fig. 4(b) corresponds to a nonresonant wavelength ($kh \approx 1.2$). We have used the same gray scale in all the contour plots presented here. The black zones in the maps correspond to relative intensities larger than a certain value. A strong enhancement of the interior field is found for the resonant case (the field is nine times larger than for any other frequency out of the resonant region), whereas in the region above the grating the field has similar values in both cases. The phase of the magnetic field inside each groove is a constant, and in resonant conditions the phase difference

between the field in adjacent grooves is π . For any other incident wavelength the phase difference takes values different from π .

We now turn to consider gratings with an increasing number of grooves per period. The geometrical parameters are kept the same as in Fig. 2(b). In Fig. 5 we plot the specular efficiency versus kh for structures with four, five, six, and seven cavities. The insets in each figure represent the resonant modes of the structure. For symmetry reasons, we expected the number of resonances in the cases of four and three grooves to be the same. This can be observed by comparing Figs. 2(b) and 5(a), where there is only one resonance. In the case of four grooves, the fields inside both central grooves must be equal (same amplitude and phase), and there can only be a phase difference of π between the fields of the external and the central grooves. Therefore, the only possible resonant configuration is [+-+]. In the case of an even number of grooves, we call this kind of resonance π resonance, although the phase difference between the central grooves is 0 and not π . Since the phase is the same in both central grooves, the resonant peak is wider and the quality factor of this resonance is smaller than that of the threegroove case.

If we add one more cavity to the period (N=5), we observe that there is a new peak in the efficiency curve [Fig. 5(b)]. For five grooves, a phase difference of π between every pair of adjacent grooves is allowed, and the peak corresponding to the π resonance becomes thinner than in the previous cases. Consequently, we get a better quality resonance and a stronger intensification of the field inside the cavities [see Fig. 6(b)]. The π resonance corresponds to the value of kh that is closer to $\pi/2$. For six grooves per period [Fig. 5(c)], we observe a behavior similar to that of the fourgroove structure: the number of resonances remains the same as in the five-groove case, but the peaks get wider and their quality decreases [Fig. 6(c)]. In Fig. 5(d) we show the specular efficiency for a grating with seven grooves in the period. A new peak appears and the π resonance is now closer to $\pi/2$ and is slightly wider than that corresponding to the fivegroove case. Notice that in this case the corrugation covers more than half a period.

We have stated that when the π resonance is sharper the intensification of the field inside the cavities is stronger. This feature can be observed in Fig. 6: the interior field is much stronger for an odd number of grooves [Figs. 6(b) and 6(d)] than for an even number [Figs. 6(a) and 6(c)]. It should be mentioned that the maximum value of the relative interior field in Fig. 6(b) is about four times larger than the one in Fig. 6(a). In addition, as the number of grooves is increased, the coupling between them competes with the edge effect, and this produces a narrowing of the zone between two zeros of the external field. In Figs. 7(a) and 7(b) we compare the relative fundamental amplitudes of the field in the cavities where it is more intense for N=5 and N=6, respectively. We chose the vertical scale to be the same in both figures in order to show that in the case of an odd number of grooves [Fig. 7(a)] the amplitude is almost three times as large as in the even case [Fig. 7(b)]. It can also be noted that in both cases the π resonance is dominant, and the second resonance



FIG. 8. (a) kh value corresponding to the π resonance versus N; (b) maximum relative magnetic field intensity inside the cavities versus N. The parameters of the grating are a/h=0.2, b/h=0.1, and d/h=6.

has an amplitude that is about a quarter of the amplitude of the π resonance. In Figs. 7(c) and 7(d) we show the phase differences for the same cases, and we observe that the rightmost resonance corresponds to the π resonance: for N=5the configuration is [+-++] and for N=6 it is [+-++-+].

The evolution of the kh value corresponding to the π resonance with the number of grooves for a/h=0.2, b/h=0.1, and d/h=6 is shown in Fig. 8. Notice that in this configuration when N=20 we have a simple grating of d/h=0.5, and consequently the maximum N allowed is N_{max} = 19. It can be observed that the position of the π resonance converges to a limit value, which is the same for odd and even numbers of grooves. The dependence of this limit value on the geometrical parameters of the structure is being studied. For the same configuration, in Fig. 8(b) we show the maximum relative magnetic field intensity at the π resonance, which is registered at the bottom of the central groove for an odd N, whereas for an even N the maximum intensity is found at the bottom of other cavities different from the central ones. It can be observed that the field intensity in the π resonance increases with increasing N up to N=9 for odd values and up to N=10 for even values. In both odd and even cases, N=9 and N=10 are the integers closest to $N_{max}/2$. From this value upward, the field intensity decreases, and the same effect can be observed in the example of Fig. 6. The position of this maximum can be explained as follows. When we start to fill the period with cavities, the behavior of the structure departs from that of a simple grating, which has no resonance [see Fig. 2(a)]. The behavior remains like that up to a certain value of N where the total length of the corrugated zone occupies half of the period. From there onward, if we increase the number of cavities, the structure becomes more and more like a simple grating with a period (a+b). The width of the π resonance efficiency peak increases and therefore its quality decreases and a less intense interior field is produced.

Each period of the composed grating can be considered as a resonant system. It is well known that the lowest mode of a resonant system is that in which all the elements are in phase. As the number of pairs of adjacent elements in counterphase increases, so does the energy of the mode. The most energetic mode of the system is that in which the fields in adjacent elements are in counterphase. Therefore, the most energetic mode can occur only for an odd N, due to the symmetry imposed by the normal incidence [see Figs. 7(a) and 7(c)]. On the other hand, the higher mode allowed for an even N is that in which there is only one pair of adjacent elements in phase [see Figs. 7(b) and 7(d)]. Consequently, even configurations are less energetic than odd ones.

IV. CONCLUSION

In this work we give numerical evidence for a resonant phenomenon that occurs in infinite gratings when the period is composed of several cavities. The diffraction problem was solved for the two basic polarization modes, in the particular case of rectangular grooves. We used the modal approach, which has proved to be particularly suitable for this geometry. The results show that when the incident field is p polarized significant resonances occur. These resonances are not allowed in simple infinite gratings. The resonant wavelengths are larger than those corresponding to the finite structure, which are slightly bigger than 4h. For such incident wavelengths, all the power is reflected specularly, and the electromagnetic field inside the cavities is enhanced. The best quality resonance (the π resonance) is the one in which the phases of the magnetic field in adjacent grooves are reversed. Therefore, for an odd number of grooves in the period we get a greater intensification than is obtained for an even number. For a given set of geometrical parameters, the best quality π resonance occurs when the corrugated zone occupies half a period. The dependence of this phenomenon on geometrical parameters such as width and distance between cavities is being studied, and will be the subject of future work.

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