Resonant effects in compound diffraction gratings: Influence of the geometrical parameters of the surface

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(Received 10 December 2001; published 22 May 2002)

We explore and discuss the influence of the geometrical parameters of a compound diffraction grating on the generation of π resonances, which appear when the surface is illuminated by a *p*-polarized plane wave. We consider a grating with rectangular grooves, and analyze the evolution of π resonances when depth, width, distance between grooves, and period of the grating are varied. In particular, we performed a detailed study for a grating with five grooves per period, and found that there are certain values of the geometrical parameters that optimize the enhancement of the electromagnetic field inside the corrugations. For an increasing depth of the grating, the resonant frequency verges on the value that corresponds to a finite grating. We also show numerical examples of the amplitude and phase of the electromagnetic field, where the differences in the near field for resonant and nonresonant configurations become apparent.

DOI: 10.1103/PhysRevE.65.056619 PACS number(s): 42.25.−p

I. INTRODUCTION

In a recent paper we provided numerical evidence of a resonant effect that appears in infinite periodic gratings formed by a group of grooves in each period (compound gratings) [1]. When the structure is illuminated by a *p*-polarized plane wave of certain wavelengths, the phase of the electromagnetic field inside the corrugations is distributed in such a way that a significant enhancement of the internal field is generated, while the specular efficiency is maximized.

This kind of resonance has been observed in finite structures comprising several longitudinal cavities, such as slotted cylinders [2,3] and rectangular grooves [4]. As shown in the references above, when a π resonance is excited, the structure behaves like a superdirective antenna, and the internal electromagnetic field is strongly intensified. In the phase resonances described in [1], the phase difference between the magnetic fields at adjacent grooves is 0 or π radians.

Phase resonances could then be added to the list of already known anomalies that occur in infinite gratings. These anomalies can be classified depending on their origin: (i) the excitation of surface polaritons in metallic shallow gratings [5–8]; (ii) Rayleigh anomalies, that occur when a new diffracted order appears [7]; (iii) the surface shape resonances, which are strongly dependent on the particular profile of the grooves and influence the reflected pattern mostly when the cavities are deep (see [9–13] for lamellar profiles and [14,15] for multivalued profiles).

The π resonances in infinite compound gratings could be used in practical applications involving selective processes, such as polarizers and filters. We are interested in exploring this possibility, and therefore investigate the behavior of the π resonances when the different parameters of the system are varied. In this paper we study in detail the resonance dependence on the geometrical parameters of the grating (width and depth of the grooves, distance between grooves, period of the grating).

To solve the problem of diffraction from a compound grating, we applied the modal method developed by Andrewartha *et. al.* [9] for perfectly conducting lamellar gratings to the case of compound gratings [1]. This method is particularly suitable for rectangular profiles of the grooves, and does not demand too much CPU time.

In Sec. II we outline the main features of the modal method applied to compound gratings. The final equations are implemented as Fortran programs to get the numerical results, shown in Sec. III. We study the case of a grating with five grooves per period, and show the dependence of the resonant peak on the depth of the grooves, the period of the grating, the width, and the distance between grooves. The results are shown and discussed. Contour plots of the internal field are shown for resonant and nonresonant configurations, and the phase of the specularly reflected field is also analyzed. In Sec. IV we give some concluding remarks.

II. MODAL APPROACH

The configuration of the diffraction problem is sketched in Fig. 1. A *p*-polarized plane wave (magnetic field in the rulings direction) of wavelength λ impinges from vacuum upon a perfectly conducting grating with a finite number of grooves (N) in each period (d). All the grooves have equal width (a) and depth (h), and the distance between grooves is b. Even though the angle of incidence θ_0 can be arbitrary, in all the examples presented here we consider $\theta_0 = 0°$.

To apply the modal method, we divide the space into two regions: one above the grating and one inside the corrugations. The basis of the modal approach is to expand the field into the interior of the cavities in its own eigenmodes, which satisfy by themselves the required boundary conditions at the walls of the grooves. On the other hand, the field for $y \geqslant 0$ is

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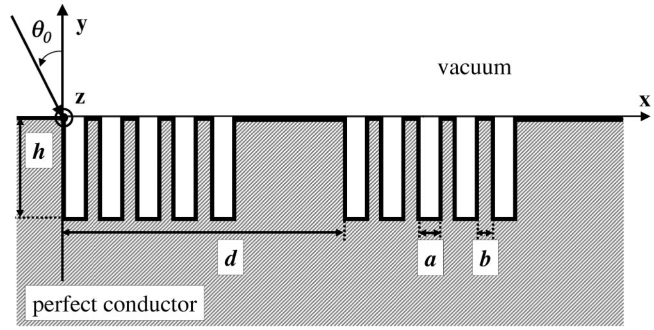

FIG. 1. Configuration of the problem.

expressed as a linear combination of plane waves, known as Rayleigh expansion. The fields in both regions are then matched imposing the continuity of the tangential magnetic field at the open zones, and the continuity of the tangential electric field along the whole period. This procedure generates two x-dependent equations that are projected on convenient bases to get an infinite system of equations for the unknown Rayleigh amplitudes and modal coefficients. The series of modes and diffracted plane waves are truncated to find the final solution of the problem by a standard matrix inversion. For details on the method and the numerical implementation, the reader is referred to Ref. [1].

III. NUMERICAL RESULTS

The response of a compound lamellar grating to a normally incident plane wave was investigated in a previous work [1]. In this reference, the study was performed for both polarizations: s (electric field parallel to the grooves) and p (magnetic field parallel to the grooves), and for a wavelength range of three only propagating orders. We found that certain resonant wavelengths associated with differences of π or 0 between the phases of the magnetic field inside the cavities only exist for p polarization and not for s polarization. Such resonances appear as sharp peaks in the curve of specular efficiency vs kh (where $k=2\pi/\lambda$ is the wave number and h is the depth of the grooves) and also in the modal amplitude vs kh.

In Fig. 2 we have plotted the specular efficiency [Fig. 2(a)], the phase difference between the fundamental modal amplitudes of adjacent grooves [Fig. 2(b)], and the fundamental modal amplitude of the central groove [Fig. 2(c)] vs kh; the period of the structure contains five grooves and the parameters are $a/h=0.2$, $b/h=0.1$, and $d/h=5.4$. In the insets in Fig. 2(a) we have schematized the electromagnetic field configurations for the phase resonances as follows: opposite (equal) signs in adjacent grooves indicate a difference of π (0) radians between the phases of the magnetic field inside the cavities. The π resonance is that in which the fields in adjacent grooves are in counterphase [$kh\approx 1.44$, see also Fig. 2(b)], whereas the peak at $kh\approx 1.38$ corresponds to the second resonance. In this example, we have three propagating orders for $kh\in[1.16,2.34]$. For $kh>2.34$ two new propagating orders appear. Notice that for $kh=2.34$, the specular efficiency has a wider peak [Fig. 2(a)], different from the other two, and the phase difference between the modal amplitudes of adjacent grooves is near 0 or π radians [Fig. 2(b)]. The analysis of the efficiency and of the phase difference at this particular wavelength seems to indicate that there is a phase resonance too. However, for $kh=2.34$ the modal amplitude has a depression [see Fig. 2(c)], whereas there are sharp peaks for the phase resonances. The appearance of a minimum in the modal amplitude does not correspond to a phase resonance. This fact suggests that to identify phase resonances it is not enough to get a peak in the efficiency and a phase difference of 0 or π radians between the phase of the magnetic field in adjacent grooves, it is also

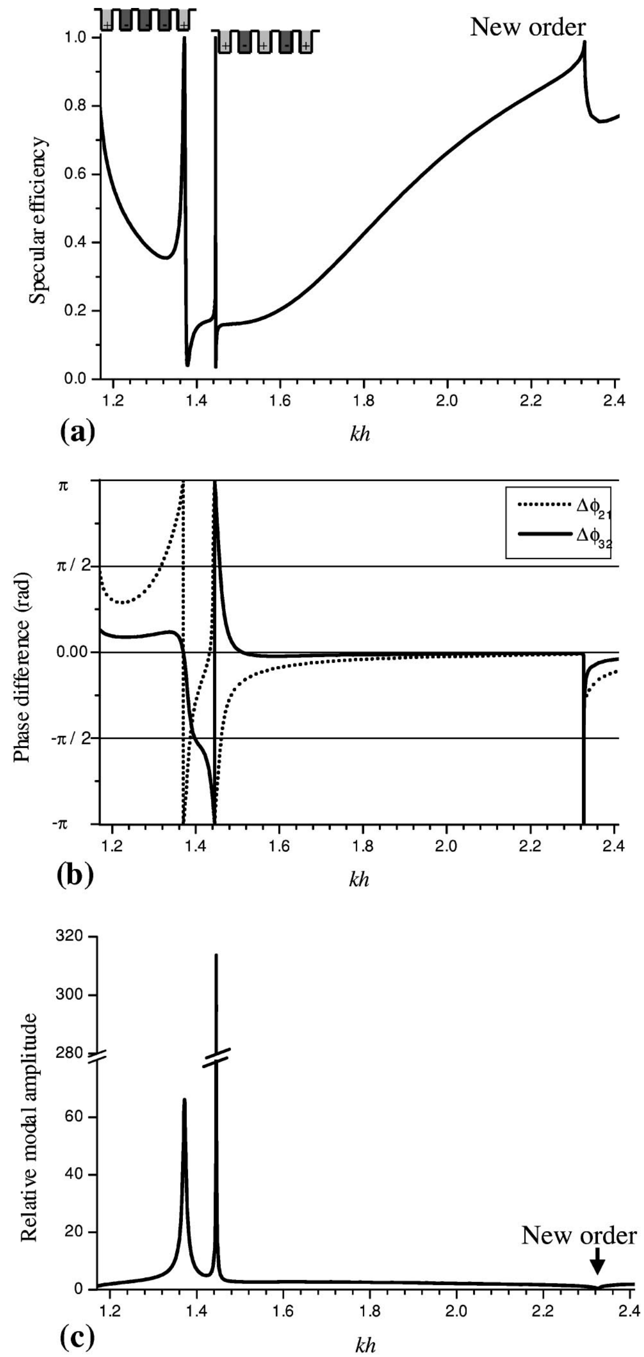

FIG. 2. Results for a grating with $N=5$, $a/h=0.2$, $b/h=0.1$, and $d/h=5.4$. (a) Specular efficiency vs kh. (b) Phase difference vs kh. (c) Relative modal amplitude vs kh.

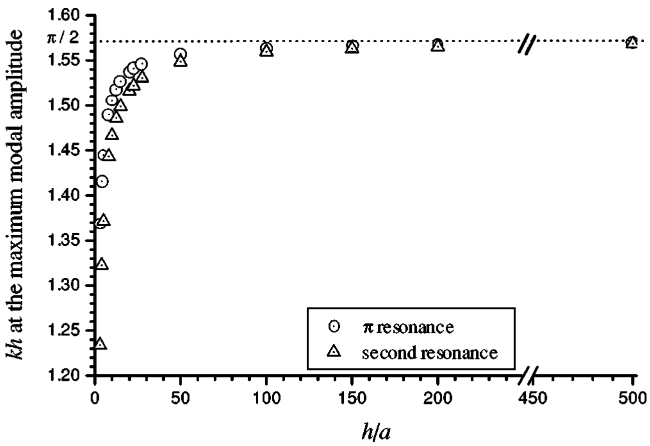

FIG. 3. kh for the maximum modal amplitude vs h/a for the π and the second resonances. The parameters of the grating are $N=5$, $b/a=0.5$, and $d/a=27$.

necessary to have an enhancement of the internal field.

Next, we study the influence of the different parameters on the position and on the quality of the resonances. Bearing in mind that phase resonances appear only for p polarization, this is the only mode considered in the examples. All the results presented correspond to normal incidence and to a grating comprising five grooves per period.

In Fig. 3 we show the effect produced by the depth of the grooves on the phase resonances. The parameters b/a and d/a were fixed: $b/a=0.5$ and $d/a=27$ for all h/a values. As the ratio h/a increases, the resonant value of kh for both the π and the second resonances become closer to each other and approach $\pi/2$ (note that to get this situation the grooves must be very deep). In such a limit case the electromagnetic field tends to be confined inside the grooves and then the value of the resonant wavelength is $4h$. This effect can be observed in Fig. 4, where we show a contour plot of the magnetic field in the vicinity of the grooves, for two values of h/a:8 [Fig. 4(a)] and 500 [Fig. 4(b)] and $b/a=0.5$ and $d/a=27$. Since $d/\lambda_{resonant}<1$, there is only one propagating order in both cases. Even though the saturation value is the same for both figures, in Fig. 4(b) the maximum magnetic field is 40 times as intense as in Fig. 4(a). For $h/a=8$ [Fig. 4(a)] $\lambda_{resonant}\sim 4.217h$, whereas for $h/a=500$ [Fig. 4(b)] $\lambda_{resonant}\sim 4.003h$. We observe that the effect produced by the corrugation on the near external field tends to be negligible while h increases.

In Fig. 5 we show the relative modal amplitude vs kh for several values of h/a. The other parameters are the same as those of Figs. 3 and 4. It can be observed that the intensification of the internal field for both the π and the second resonances increases with the ratio h/a. This is consistent with the results shown in Figs. 3 and 4. We have also observed that for $h/a<3$ (not shown in Fig. 5) the quality of the resonance decreases and the peak of specular efficiency becomes wider and lower than unity. The quality of the resonance can be evaluated not only by its maximum modal amplitude but also by the width of the peak. Better quality resonances are observed when the two-phase resonances existing for $N=5$ become closer to each other, which is the case for large values of h/a. Therefore, we conclude that the quality of the resonance is strongly dependent on the h/a ratio.

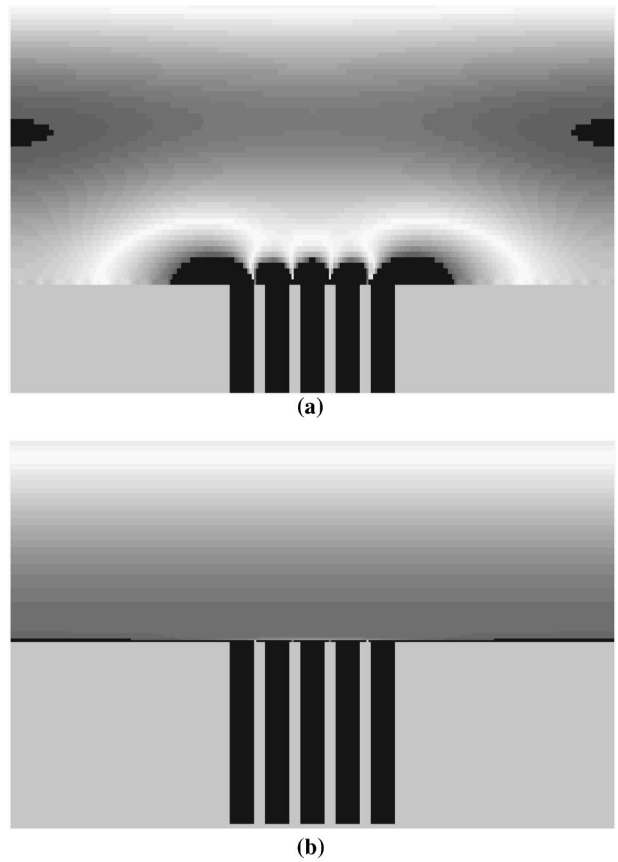

FIG. 4. Contour plots of the relative magnetic field in the vicinity of the structure with $N=5$, $b/a=0.5$, and $d/a=27$ for two resonant situations. (a) $h/a=8$; (b) $h/a=500$.

To study the influence of the period on the resonant wavelength, we varied the rate of the corrugated zone in relation to the flat one (occupancy factor) by changing the period d and setting $a/h=0.2$ and $b/h=0.1$. These results are shown in Fig. 6. Note that the position of the kh value for the π resonance remains almost constant, and its relative variation is less than 5×10^{-3} [the vertical scales of Fig. 6(a) and Fig. 3 are the same]. Despite this, the maximum field intensity

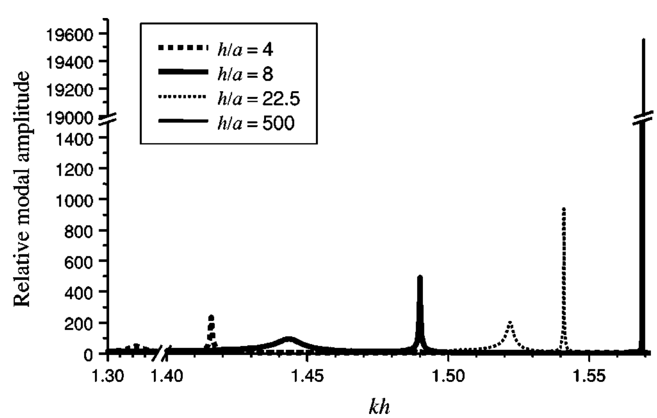

FIG. 5. Relative modal amplitude of the fundamental mode vs kh for several values of h/a. The parameters of the grating are $N=5$, $b/a=0.5$, and $d/a=27$.

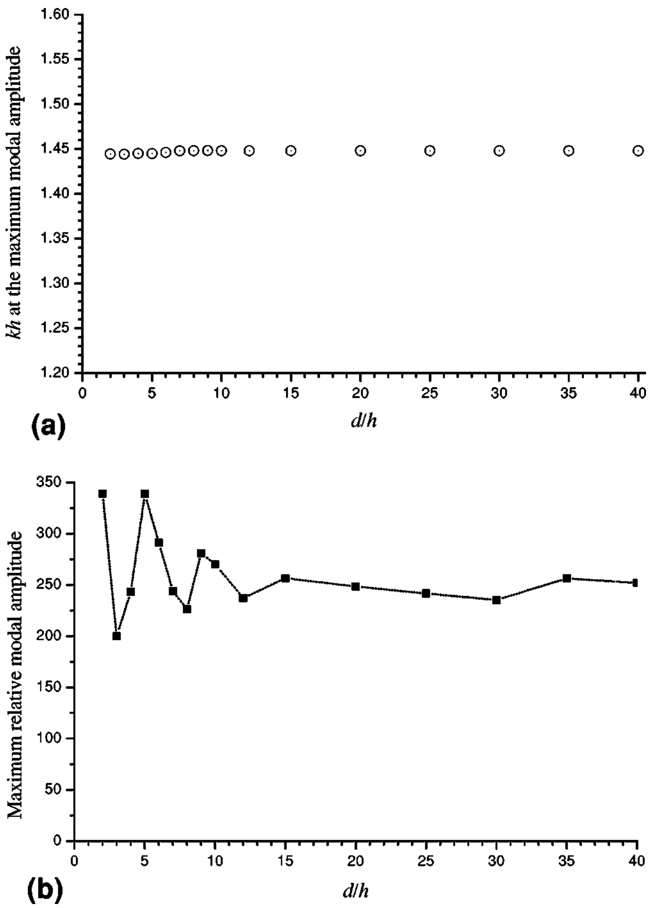

FIG. 6. (a) kh for the maximum modal amplitude corresponding to the π resonance vs d/h. (b) The maximum relative amplitude of the fundamental mode vs d/h. The dotted line only connects the points for a better visualization. The parameters of the grating are $N=5$, $a/h=0.2$, and $b/h=0.1$.

[Fig. 6(b)] depends strongly on the relative variation of the period for occupancy factors greater than 10%, which correspond to $d/h<15$ in Fig. 6(b) (the dotted line connects the points for a better visualization). Owing to this result and to our interest in considering occupation factors greater than 10%, in what follows we analyze the influence of the width and the separation between grooves (a/h and b/h) with a fixed occupancy factor.

Next, we study the dependence of the π resonance (its kh and the field intensification) on a/h and on b/h separately. A change in a/h with a fixed d/h implies a change in the occupancy factor, and then, variations of the modal amplitude could be produced by a variation of a/h as well as of the occupation factor. Therefore, we adjust d/h in Figs. 7 and 8 so that the occupation factor remains constant when varying a/h or b/h. In Fig. 7 we show the dependence of the kh value corresponding to the maximum relative modal amplitude in the π resonance, on the relative width of the grooves [Fig. 7(a)], and on the relative separation between grooves [Fig. 7(b)]. In both cases the symbols correspond to the numerical results and $d/h=18(a+b)/h$, so that the occupancy factor is the same. In Fig. 7(a) each solid line is a second-order polynomial fit for a given value of b/h, whereas in Fig. 7(b) each line corresponds to a third-order polynomial fit for

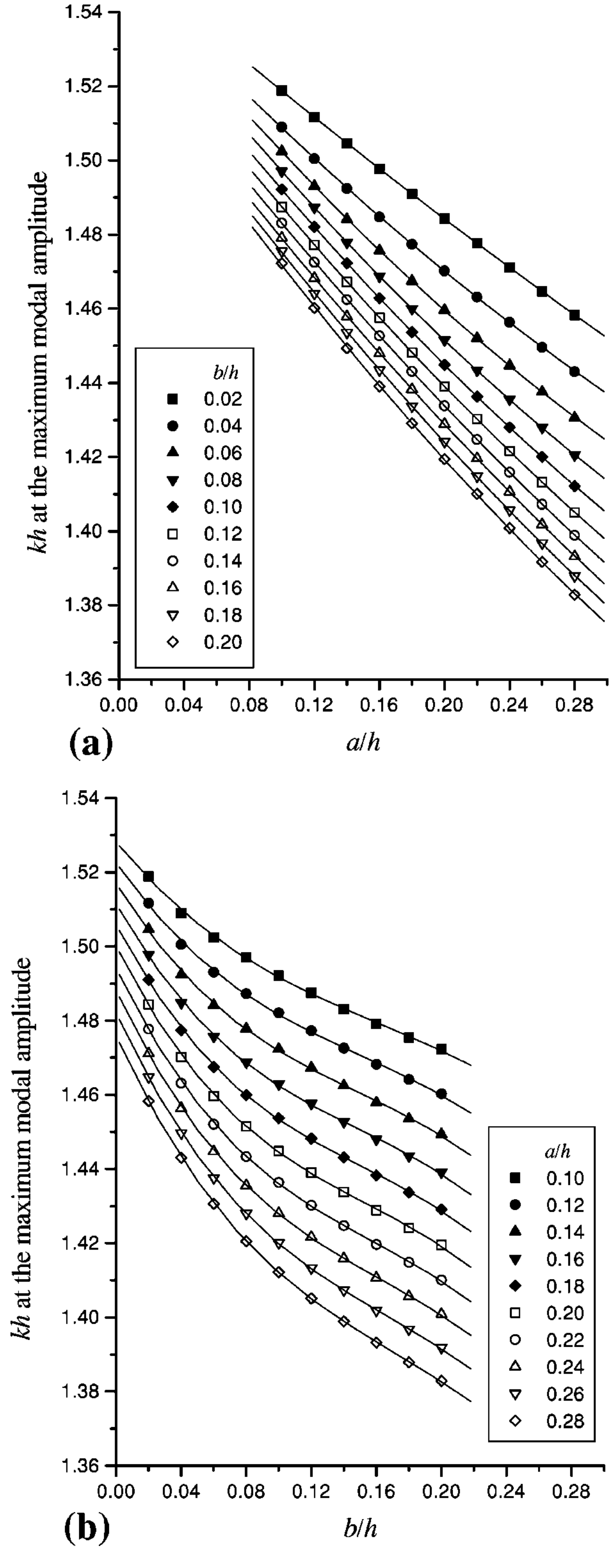

FIG. 7. (a) kh for the maximum modal amplitude at the π resonance vs a/h for several values of b/h. The solid lines are the best fits with a second-order polynomial. (b) kh for the maximum modal amplitude at the π resonance vs b/h for several values of a/h. The solid lines are the best fits with a third-order polynomial. The parameters of the grating are $d/h=5.4$ and $N=5$.

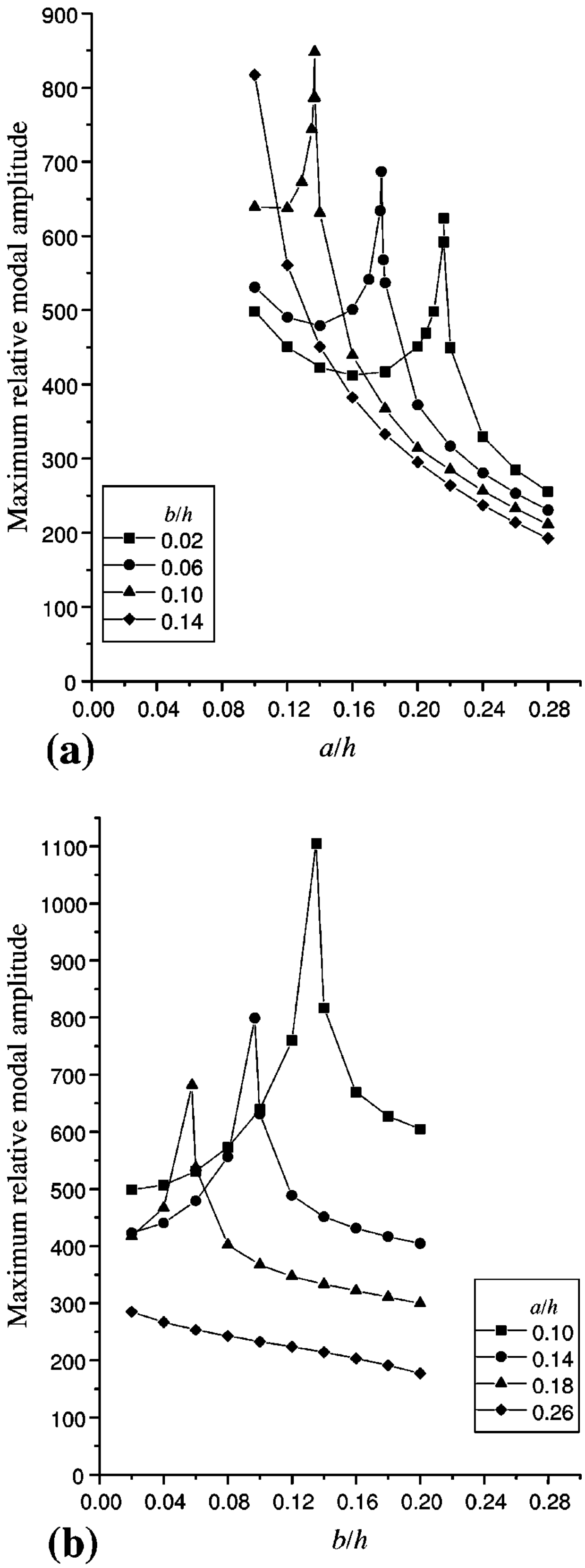

FIG. 8. (a) Maximum relative amplitude of the fundamental mode at the π resonance vs a/h for several values of b/h. (b) The maximum relative amplitude of the fundamental mode at the π resonance vs b/h for several values of a/h. The parameters of the grating are $d/h=5.4$, $N=5$.

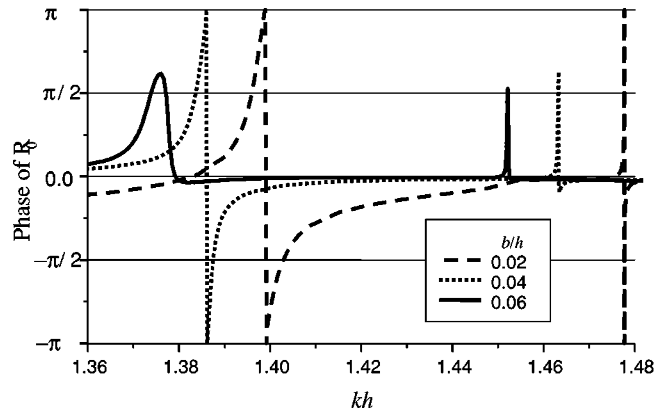

FIG. 9. Phase of the specular Rayleigh coefficient vs kh for several values of b/h. The parameters of the grating are $N=5$, $a/h=0.22$, and $d/h=18(a+b)/h$.

a constant value of a/h. We can see that for each b/h, the kh resonant value becomes closer to $\pi/2$ while a/h decreases. However, the limit value for a/h tending to 0 depends on b/h. A similar behavior is observed in Fig. 7(b) for decreasing values of b/h.

It is well known that for normal incidence, the number of propagating orders is $2[d/\lambda]+1$, where the brackets correspond to the greatest integer in d/λ. Since the π resonance takes place at $kh<\pi/2$, then $\lambda/h>4$. In the examples considered in Fig. 7, d/λ is always less than 2, and so we have one propagating order for $d/h<4$ and three propagating orders for $d/h>4$. This can influence the response of the grating at a resonance.

Next, we analyze the influence of a/h and b/h on the maximum relative modal amplitude. Figures 8(a) and 8(b) represent these dependences, and they correspond to some cases already studied in Figs. 7(a) and 7(b). We first consider Fig. 8(a). According to Fig. 5 (in the range of kh considered there is only one propagating order), we expected an improvement of the quality of the resonance as a/h decreases. However, in Fig. 8(a) we observe that the curves show quite a different behavior. Starting from $a/h=0.28$ (where there are three propagating orders for all values of b/h considered) and going downwards, the modal amplitude grows up to a maximum, which is always found in the value of a/h where the diffracted orders 1 and -1 propagate at grazing angles. From that point onwards, there is only one propagating order, and the relative modal amplitude decreases up to a certain value of a/h, where it starts to increase again. As we expected, the modal amplitude increases when a/h falls to zero. Therefore, we conclude that if we keep the number of propagating orders fixed, we obtain the best quality of the resonance for the minimum value of a/h.

The curves of maximum modal amplitude vs b/h [Fig. 8(b)] show that if there are three propagating orders, a decrease in b/h improves the resonance. On the other hand, if there is only one propagating order, a decrease in b/h worsens the quality of the resonance.

In Fig. 9 we have analyzed the phase of the specular Rayleigh coefficient vs kh. Even though this is generally a smooth function, in the vicinity of a resonance the phase has a steep change or a peak. A steep change appears when there is only one propagating order (dashed line, $kh \approx 1.4$) or when two of the three orders are almost grazing (dashed line, $kh \approx 1.48$; dotted line, $kh \approx 1.386$). On the other hand, a peak appears when there are three or more propagating orders (dotted line, $kh \approx 1.465$; solid line, $kh \approx 1.375$ and 1.45). Notice that the first group of three resonances correspond to what we call second resonance (see Fig. 2), whereas the second group are the π resonances. It can also be observed that the quality of the resonances is related to the width of the peak in the phase of the specular Rayleigh coefficient.

Finally, in Fig. 10 we show the contour plots of the magnetic field in the vicinity of the structure corresponding to four situations in which $b/a = 0.5$, $d/a = 27$, $\lambda/a = 17.75$, and $h/a = 3$, 4, 5, 8. Taking into account these parameters, we have three propagating orders in all the figures. However, the wavelength is resonant only in Fig. 10(b). In this case the efficiency of the specular order is ≈ 1, and in the far field we see the interference pattern between the incident and the reflected waves. A similar effect can be observed in Fig. 10(d), where the depth of the grooves is approximately half of a wavelength, which is close to that of the next π resonance ($kh \approx 3\pi/2$). On the other hand, a different behavior can be observed in Figs. 10(a) and 10(c), where the specular efficiency is less than 1. Therefore, the interference pattern of four waves is obtained. The vertical shift of the pattern is due to the variation of the phase of the Rayleigh coefficients. It must be noticed that the internal field in the resonant case [Fig. 10(b)] is strongly intensified and the amplitudes of the evanescent waves are sufficiently large to modify the interference pattern close to the structure.

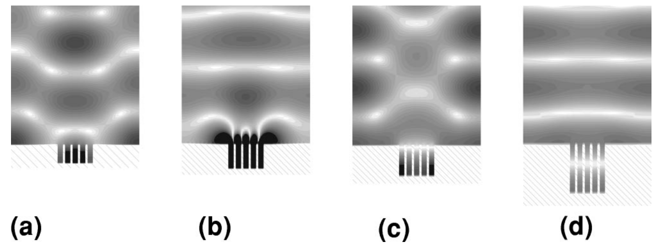

FIG. 10. Contour plots of the relative magnetic field in the vicinity of the structure with $N = 5$, $b/a = 0.5$, $d/a = 27$, and $\lambda/a = 17.75$ for four different situations: (a) $h/a = 3$; (b) $h/a = 4$ (resonant situation); (c) $h/a = 5$; (d) $h/a = 8$.

IV. CONCLUSION

In this paper we have analyzed the phase resonances that take place when a *p*-polarized plane wave impinges on a diffraction grating comprising several grooves per period. We considered a perfectly conducting grating with rectangular grooves. The study was focused on finding the influence of the geometrical parameters of the grating, taken separately, on the characteristics of the resonances. We found that when a phase resonance occurs, both the reflected efficiency and the amplitude of the field inside the grooves are maximized, and the phase difference between the fields at adjacent grooves is 0 or π radians. If the number of propagating orders is fixed, an increase in the depth of the grooves produces a more significant enhancement of the internal field and a narrowing of the efficiency peak. This improves the quality of the resonance. We also studied the dependence of the π resonance wavelength on the width and on the distance between grooves for a constant occupancy factor, and found that the resonant wavelength approaches $4h$ when these parameters are decreased. We have shown that the phase of the specular Rayleigh coefficient also gives information about the phase resonances, and that the near field is modified when the incident plane wave has a resonant wavelength.

Since we are interested in the application of these resonances in selective devices, we are now modeling a more realistic metallic grating with finite conductivity. The results of this study will be the subject of a future work.

ACKNOWLEDGMENTS

This work has been supported by Universidad de Buenos Aires (UBA) under Grant No. JX76, and by Agencia Nacional de Promoción Científica y Tecnológica (ANPCyT) under Grant No. PICT98-4457.

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