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Optics Communications 258 (2006) 90-96

Optics Communications

www.elsevier.com/locate/optcom

# Application of the differential method to uniaxial gratings with an infinite number of refraction channels: Scalar case

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Received 10 May 2005; received in revised form 25 July 2005; accepted 26 July 2005

#### Abstract

The differential method (also called the C method) is applied to the diffraction of linearly polarized plane waves at a periodically corrugated boundary between vacuum and a linear, homogeneous, uniaxial, dielectric-magnetic medium characterized by hyperbolic dispersion equations. Numerical results for sinusoidal gratings are presented and compared with those obtained by means of the Rayleigh method, showing that both the differential method and the Rayleigh method can fail to give adequate results for gratings supporting an infinite number of refracted Floquet harmonics.

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Keywords: Anisotropy; Diffraction; Grating; Negative refraction; Elliptic dispersion equation; Hyperbolic dispersion equation

# 1. Introduction

This communication is in the context of materials exhibiting negative-phase-velocity characteristics [1,2]. In such materials, the angle between the phase velocity vector and the time-averaged Poynting vector is obtuse [3], thereby leading to interesting and exploitable effects [4]. Our focus is on surface-relief gratings made of materials with anisotropic dielectric and magnetic properties.

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<sup>0030-4018/\$ -</sup> see front matter @ 2005 Elsevier B.V. All rights reserved. doi:10.1016/j.optcom.2005.07.067

### 2. Boundary value problem

Let us consider the diffraction of plane waves at a periodically corrugated boundary between vacuum and a linear, homogeneous, uniaxial, dielectricmagnetic medium. The relative permeability and permittivity tensors of the diffracting medium share the same optic axis denoted by the unit vector  $\hat{c}$ , and their four eigenvalues are denoted by  $\epsilon_{\perp\parallel}$  and  $\mu_{\perp\parallel}$ , where the subscript  $\perp$  indicates the element of the tensor in the plane perpendicular to the optic axis and the subscript || corresponds to the element along it. We are interested in both constitutive tensors being indefinite, in the sense that they have positive and negative eigenvalues (i.e.,  $\epsilon_{\perp}\epsilon_{\parallel} < 0$  and  $\mu_{\parallel}\mu_{\parallel} < 0$ ). Planewave propagation is then characterized by hyperbolic dispersion equations, which leads to the refraction of an incident plane wave into an infinite set of propagating Floquet harmonics [5]. Materials with such properties are rapidly becoming possible [6,7] and can be expected to play a significant role in flat lenses made with metamaterials [8].

In order to understand their unusual characteristics, let us begin with a Cartesian coordinate system, chosen so that the x- and z-axis are perpendicular and parallel respectively to the grating grooves. A grating with sinusoidal profile  $g(x) = 0.5h\cos(2\pi x/d)$  (h is the groove depth and d is the grating period) is illuminated from the vacuous side by either an s or a p polarized plane wave, with its wavevector lying on the mean section of the grating (xy plane). The optic axis  $\hat{c} = (c_x, c_y, c_z)$  lies in the incidence plane  $(c_z = 0)$ , forming an angle  $\theta_c$  with the y-axis; hence, the diffracted plane waves have the same linear polarization state as the incident plane wave. An  $\exp(-i\omega t)$  time-dependence is assumed, with  $\omega$  as the angular frequency. The vacuum wavenumber and wavelength are denoted by  $k_0$  and  $\lambda_0$ .

### 3. Dispersion equations

The dispersion equations for the Floquet harmonic of order  $n \in \mathbb{Z}$  in the diffracting medium are as follows [9]:

$$\begin{pmatrix} \epsilon_{\perp}c_{x}^{2} + \epsilon_{\parallel}c_{y}^{2} \end{pmatrix} \begin{pmatrix} \beta_{n}^{(E)} \end{pmatrix}^{2} + 2(\epsilon_{\parallel} - \epsilon_{\perp})c_{x}c_{y}\alpha_{n}\beta_{n}^{(E)} \\ + \alpha_{n}^{2} \begin{pmatrix} \epsilon_{\perp}c_{y}^{2} + \epsilon_{\parallel}c_{x}^{2} \end{pmatrix} = k_{0}^{2}\mu_{\perp}\epsilon_{\perp}\epsilon_{\parallel},$$
(1)

$$\begin{pmatrix} \mu_{\perp}c_{x}^{2} + \mu_{\parallel}c_{y}^{2} \end{pmatrix} \left(\beta_{n}^{(M)}\right)^{2} + 2(\mu_{\parallel} - \mu_{\perp})c_{x}c_{y}\alpha_{n}\beta_{n}^{(M)} \\ + \alpha_{n}^{2}\left(\mu_{\perp}c_{y}^{2} + \mu_{\parallel}c_{x}^{2}\right) = k_{0}^{2}\epsilon_{\perp}\mu_{\perp}\mu_{\parallel}.$$
 (2)

Eqs. (1) and (2) hold for waves of the electric and magnetic types, respectively, and need to be solved for  $\beta_n^{(j)}$  (j = E, M); whereas  $\alpha_n = k_0 \sin \theta_0 + n \frac{2\pi}{d}$  with  $\theta_0 \in [-\pi/2, \pi/2]$  being the angle between the incident wavevector and the *y*-axis.

For illustration, let us consider the two following sets of constitutive scalars:

- *Case I.*  $\epsilon_{\perp} = -2.1$ ,  $\epsilon_{\parallel} = 1.9$ ,  $\mu_{\perp} = 1.3$  and  $\mu_{\parallel} = -1.6$ ;
- Case II.  $\epsilon_{\perp} = 2.1$ ,  $\epsilon_{\parallel} = -1.9$ ,  $\mu_{\perp} = -1.3$  and  $\mu_{\parallel} = 1.6$ .

The dispersion Eqs. (1) and (2) then describe hyperbolas, as shown in Fig. 1 for  $\lambda_0 = 1.5d$ ,



Fig. 1. Reciprocal space map for  $\epsilon_{\perp} = \pm 2.1$ ,  $\epsilon_{\parallel} = \pm 1.9$ ,  $\mu_{\perp} = \pm 1.3$  and  $\mu_{\parallel} = \pm 1.6$  (Cases I (upper sign) and II (lower sign)) and for  $\theta_c = 60^\circ$ .  $k_x$  and  $k_y$  denote, respectively, the *x* and *y* component of the wavevectors. The horizontal gray, doubled-arrow indicates the value of  $\lambda_0 = 1.5d$  and the black arrows indicate the incident and the specularly reflected wavevectors. Wavevectors for n = 1 for Case I and n = -1 for Case II, both corresponding to orders of the electric type (p polarization), are plotted.

wherein we have plotted the reciprocal space maps for both cases. The circle refers to Floquet harmonics in the medium of incidence, the inner hyperbolas correspond to harmonics of the electric type and the outer ones correspond to harmonics of the magnetic type in the diffracting medium. Both  $\beta_n^{(E)}$  and  $\beta_n^{(M)}$ are real-valued  $\forall n \in \mathbb{Z}$ . Thus, in contrast to the case of gratings made of conventional materials, for which the refracted field consists of a few propagating and the remaining evanescent harmonics, gratings of materials with indefinite constitutive tensors may refract a plane wave into an infinite number of propagating harmonics. This unusual feature requires that close attention be paid when available theoretical methods are applied for gratings of these kinds of materials.

### 4. Differential method

For gratings made of isotropic materials exhibiting negative-phase-velocity characteristics, several commonplace grating methods have been applied. These methods include the perturbation method [10], the Rayleigh method [11], and the differential method [12,13]. The dispersion equations were elliptic, and all methods performed as well as for gratings made of isotropic materials with positive-phase-velocity characteristics.

Turning our attention to anisotropic gratings exhibiting negative refraction, we commenced with an application of the Rayleigh method [5]. Although it yielded satisfactory results for very shallow sinusoidal gratings, the method completely failed for deeper gratings (even within the expected validity range of the Rayleigh hypothesis), giving non-convergent results. If this lack of convergence were related to the existence of an infinite number of refraction channels, the problem would have to be shared by other available theoretical methods for gratings. Therefore, we decided to investigate the applicability of the widely used differential method of Chandezon et al. [14–18], also known as the C method.

For the grating configuration chosen, the diffraction of s and p plane waves can be considered separately. Starting from the Maxwell equations, and using the change of variables v = x and u = y - a(x), we obtain a pair of differential equations

$$\begin{bmatrix} k_0^2 A_0 + A_1 \frac{\partial^2}{\partial v^2} & 0\\ 0 & 1 \end{bmatrix} \begin{bmatrix} F\\ F' \end{bmatrix}$$
$$= \begin{bmatrix} i A_1 \left( \frac{\partial}{\partial v} \dot{a} + \dot{a} \frac{\partial}{\partial v} \right) - i A_3 \frac{\partial}{\partial v} & A_2 + A_1 \dot{a}^2 - A_3 \dot{a} \\ 1 & 0 \end{bmatrix}$$
$$\times \frac{1}{i} \frac{\partial}{\partial u} \begin{bmatrix} F\\ F' \end{bmatrix}, \tag{3}$$

where  $\dot{a}=da/dv$ ,  $F = E_z$  ( $F = H_z$ ) for s (p) polarization, and  $F' \equiv -i\partial F/\partial u$ . Whereas

$$\begin{array}{l} A_{0} = \mu_{\perp} \\ A_{1} = \frac{\epsilon_{\parallel}c_{x}^{2} + \epsilon_{\perp}c_{y}^{2}}{\epsilon_{\parallel}\epsilon_{\perp}} \\ A_{2} = \frac{\epsilon_{\perp}c_{x}^{2} + \epsilon_{\parallel}c_{y}^{2}}{\epsilon_{\parallel}\epsilon_{\perp}} \\ A_{3} = \frac{2(\epsilon_{\parallel} - \epsilon_{\perp})c_{x}c_{y}}{\epsilon_{\perp}\epsilon_{\parallel}} \end{array}$$

$$\tag{4}$$

for p polarization, the expressions for  $A_j$  (j = 0, 3)for s polarization are obtained from Eq. (4) after substituting  $\epsilon_{\parallel} \rightarrow \mu_{\parallel}$  and  $\epsilon_{\perp} \rightarrow \mu_{\perp}$ . Parenthetically, Eq. (3) reduces to Eq. (8) of Li et al. [18] when  $\epsilon_{\perp} = \epsilon_{\parallel}$  and  $\mu_{\perp} = \mu_{\parallel}$ . Subsequent steps of the differential method are skipped as they are the same as for isotropic gratings [14,18]. Most notably, one has to restrict  $|n| \leq N$  for computations.

#### 5. Numerical results

Numerical results with the differential and the Rayleigh methods were first compared for  $\epsilon_{\perp} = \mp 2.1$ ,  $\epsilon_{\parallel} = \pm 1.9$ ,  $\mu_{\perp} = \pm 1.3$ ,  $\mu_{\parallel} = \mp 1.6$ , h/d = 0.1,  $\lambda_0 = 1.5d$ , and  $\theta_0 = 27^\circ$  [5]. Tables 1 (for  $\hat{c} = \hat{x}$ ) and 2 (for  $\hat{c} = \hat{y}$ ) show the computed reflection and refraction efficiencies. We used Floquet harmonics of orders  $|n| \leq 11$ , which sufficed to ensure that the principle of conservation of energy was satisfied to an error of 1 ppm. No significant difference between the results from the two methods was observed.

Both tables show that the zeroth-order (i.e., specular) harmonic (refracted in Table 1 or reflected in Table 2) carries a large part of the energy incident onto the grating whereas the higher-order efficiencies are small, a fact that ensures convergence, Table 1

Reflection (*r*) and refraction (*t*) efficiencies for a sinusoidal grating for both linear polarization states of the incident plane wave (s and p);  $\hat{c} = \hat{x}$ ,  $\epsilon_{\perp} = \pm 2.1$ ,  $\epsilon_{\parallel} = \pm 1.9$ ,  $\mu_{\perp} = \pm 1.3$ ,  $\mu_{\parallel} = \pm 1.6$ , the upper (lower) sign corresponds to Case I (II); h/d = 0.1,  $\lambda_0 = 1.5d$  and  $\theta_0 = 27^\circ$ . The differential method was used with  $|n| \leq 11$ 

Efficiency	s (I)	p (I)	s (II)	p (II)
$r_0$	$0.1337 \times 10^{-1}$	$0.1505 \times 10^{-3}$	$0.1929 \times 10^{-1}$	$0.1355 \times 10^{-2}$
t_2	$0.3427 \times 10^{-2}$	$0.3465 \times 10^{-3}$	$0.4381 \times 10^{-4}$	$0.3215 \times 10^{-2}$
$t_{-1}$	$0.6386 \times 10^{-1}$	$0.2394 \times 10^{-2}$	$0.8579 \times 10^{-3}$	$0.7690 \times 10^{-1}$
$t_0$	0.8313	0.9821	0.9573	0.8475
$t_1$	$0.8052 \times 10^{-1}$	$0.1443 \times 10^{-1}$	$0.2139 \times 10^{-1}$	$0.6632 \times 10^{-1}$
$t_2$	$0.6416 \times 10^{-2}$	$0.4874 \times 10^{-3}$	$0.1050 \times 10^{-2}$	$0.4164 \times 10^{-2}$

Table 2

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Efficiency	s (I)	p (I)	s (II)	p (II)
<i>r</i> <sub>0</sub>	0.9815	0.9526	0.9729	0.9626
$t_{-2}$	$0.3074 \times 10^{-4}$	$0.7550 \times 10^{-3}$	$0.1751 \times 10^{-3}$	$0.1163 \times 10^{-3}$
$t_{-1}$	0	0	0	0
$t_0$	0	0	0	0
$t_1$	$0.1624 \times 10^{-1}$	$0.4403 \times 10^{-1}$	$0.2633 \times 10^{-1}$	$0.3375 \times 10^{-1}$
<i>t</i> <sub>2</sub>	$0.2045 \times 10^{-2}$	$0.2226 \times 10^{-2}$	$0.5720 \times 10^{-3}$	$0.3068 \times 10^{-2}$

although there is an infinite set of refracted harmonics available. Furthermore, the specularly refracted orders of both types are of the evanescent kind, when  $\hat{c} = \hat{y}$ . Moreover, for the parameters chosen in our example, the order n = -1 of the magnetic or of the electric type (depending on the polarization of the incident wave) is also evanescent.

When the corrugation depth was increased to h/d = 0.2, we were unable to obtain convergent results, thereby confirming that the lack of convergence, already observed for the Rayleigh method, is also present when the differential method is applied.

We then examined a slightly different situation in which an infinite number of refracted harmonics propagate in the diffracting medium for s polarization, but all refracted orders are evanescent  $(\beta_n^2 < 0 \ \forall n \in \mathbb{Z})$  for p polarization. The constitutive parameters for this example are  $\epsilon_{\perp} = -2.1$ ,  $\epsilon_{\parallel} = -1.9$ ,  $\mu_{\perp} = 1.3$ ,  $\mu_{\parallel} = -1.6$ ; furthermore,  $\hat{c} = \hat{y}$ and  $\lambda_0 = 1.1d$ . As for our previous examples, the differential method performs well for shallow gratings but is inadequate for deep gratings for s polarization. On the other hand, for p polarization, results converge satisfactorily, even for gratings with h/d up to 0.3, as can be deduced from Table 3. These results indicate the connection between the lack of convergence and the existence of an infinite set of propagating Floquet harmonics in the diffracting medium.

For further investigation, we reoriented the optic axis to  $\theta_c = 60^\circ$ , the other parameters remaining the same as for Table 1. For both Cases I and II, we found that the differential method does not converge for h/d > 0.05. Results for h/d = 0.05 are presented in Tables 4–7. For p-polarized incidence, the convergence is very good for both Cases I and II (Tables 4 and 5). For s-polarized incidence, the principle of conservation of energy<sup>1</sup> is poorly satisfied for low values of N but is not satisfied as N is increased, although the efficiencies of the lower-order harmonics seem to converge. For Case II, despite the satisfaction of the principle of conservation of energy, the efficiencies of the higher-order harmonics diverge

<sup>&</sup>lt;sup>1</sup> The quantity indicated as PC in Tables 4–7 should equal unity, if the principle of conservation of energy is satisfied. The greater the value of |1 - PC|, the less satisfactory are the computed results.

Table 3

Reflection efficiencies for a sinusoidal grating with different values of h/d illuminated by a p-polarized plane wave, when  $\theta_0 = 27^\circ$ ,  $49^\circ$  and  $73^\circ$ ;  $\epsilon_{\perp} = -2.1$ ,  $\epsilon_{\parallel} = -1.9$ ,  $\mu_{\perp} = 1.3$ ,  $\mu_{\parallel} = -1.6$ ,  $\hat{c} = \hat{y}$  and  $\lambda_0 = 1.1d$ . The differential method was used with  $|n| \le 11$ 

, ·	,, <i>p</i>						
$\theta_0$	Efficiency	h/d = 0.05	h/d = 0.1	h/d = 0.2	h/d = 0.3		
27°	<i>r</i> <sub>1</sub>	$0.4128 \times 10^{-1}$	0.1966	0.1571	0.7824		
	<i>r</i> <sub>0</sub>	0.9587	0.8034	0.8429	0.2176		
49°	<i>r</i> <sub>1</sub>	$0.2854 \times 10^{-1}$	$0.6670 \times 10^{-1}$	$0.4695 \times 10^{-1}$	0.2515		
	$r_0$	0.9715	0.9333	0.9530	0.7485		
73°	$r_1$	$0.1803 \times 10^{-1}$	$0.6595 \times 10^{-1}$	0.1563	$0.3767 \times 10^{-1}$		
	<i>r</i> <sub>0</sub>	0.9820	0.9341	0.8437	0.9623		

Table 4

Reflection (r) and refraction (t) efficiencies for a sinusoidal grating with h/d = 0.05 for Cases I and II and for a p-polarized incident plane wave. Other parameters are  $\theta_0 = 27^\circ$ ,  $\theta_c = 60^\circ$  and  $\lambda_0 = 1.5d$ ; N = 9 for Case I and N = 21 for Case II

Case	<i>r</i> <sub>0</sub>	$t_{-1}$	$t_0$	$t_1$	PC
I II	$0.2693 \times 10^{-1}$ 0.3284 × 10 <sup>-1</sup>	$0.1221 \times 10^{-2}$ 0.1313 × 10^{-1}	0.9687 0.8926	$0.3119 \times 10^{-2}$ 0.5189 × 10^{-1}	1.0000
II	$0.3284 \times 10^{-1}$	$0.1221 \times 10^{-1}$ $0.1313 \times 10^{-1}$	0.8926	$0.5189 \times 10^{-1}$	1.0001

Table 5

Same as Table 4, but for  $\theta_0 = 49^\circ$ 

Case	<i>r</i> <sub>0</sub>	$t_{-1}$	$t_0$	$t_1$	PC
I II	$\begin{array}{c} 0.1438 \times 10^{-2} \\ 0.5911 \times 10^{-3} \end{array}$	$\begin{array}{c} 0.3632 \times 10^{-3} \\ 0.2974 \times 10^{-1} \end{array}$	0.9954 0.8816	$\begin{array}{c} 0.2528 \times 10^{-2} \\ 0.6919 \times 10^{-1} \end{array}$	1.0000 1.0002

Table 6

Reflection (r) and refraction (t) efficiencies for a sinusoidal grating with h/d = 0.05 for Cases I and II and for a s-polarized incident plane wave. Several values of N are considered. Other parameters are  $\theta_0 = 27^\circ$ ,  $\theta_c = 60^\circ$  and  $\lambda_0 = 1.5d$ 

Case	Efficiency	N = 7	N = 9	N = 11	N = 13	N = 15
Ι	$r_0$	$0.5537 \times 10^{-2}$	$0.5538 \times 10^{-2}$	$0.5538 \times 10^{-2}$	(*)	(*)
	$t_{-2}$	$0.1081 \times 10^{-2}$	$0.1084 \times 10^{-2}$	$0.1085 \times 10^{-2}$		
	$t_{-1}$	$0.8720 \times 10^{-2}$	$0.8706 \times 10^{-2}$	$0.8704 \times 10^{-2}$		
	$t_0$	0.8759	0.8760	0.8760		
	$t_1$	$0.8320 \times 10^{-1}$	$0.7819 \times 10^{-1}$	$0.7866 \times 10^{-1}$		
	PC	1.0636	1.0790	1.1121		
II	$r_0$	$0.2622 \times 10^{-2}$				
	$t_{-3}$	$0.1509 \times 10^{-2}$	$0.1405 \times 10^{-3}$	$0.3417 \times 10^{-3}$	$0.1717 \times 10^{-3}$	$0.1979 \times 10^{-3}$
	t_2	$0.4606 \times 10^{-3}$	$0.8343 \times 10^{-3}$	$0.7381 \times 10^{-3}$	$0.7489 \times 10^{-3}$	$0.7478 \times 10^{-3}$
	$t_{-1}$	$0.7260 \times 10^{-2}$	$0.7201 \times 10^{-2}$	$0.7204 \times 10^{-2}$	$0.7203 \times 10^{-2}$	$0.7203 \times 10^{-2}$
	$t_0$	0.9847	0.9847	0.9847	0.9847	0.9847
	$t_1$	$0.4430 \times 10^{-2}$	$0.4428 \times 10^{-2}$	$0.4428 \times 10^{-2}$	$0.4428 \times 10^{-2}$	$0.4428 \times 10^{-2}$
	PC	1.0009	1.0010	1.0013	1.0019	1.0033

(\*) Not shown since the differential method fails to give acceptable results.

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Efficiency	N = 7	N = 9	N = 11	N = 13	N = 15		
<i>r</i> <sub>0</sub>	$0.2633 \times 10^{-1}$						
<i>t</i> <sub>-3</sub>	$0.2413 \times 10^{-3}$	$0.2125 \times 10^{-4}$	$0.5522 \times 10^{-4}$	$0.3322 \times 10^{-4}$	$0.3649 \times 10^{-4}$		
<i>t</i> <sub>-2</sub>	$0.1083 \times 10^{-3}$	$0.1695 \times 10^{-3}$	$0.1569 \times 10^{-3}$	$0.1581 \times 10^{-3}$	$0.1580 \times 10^{-3}$		
$t_{-1}$	$0.2317 \times 10^{-2}$	$0.2309 \times 10^{-2}$	$0.2309 \times 10^{-2}$	$0.2309 \times 10^{-2}$	$0.2309 \times 10^{-2}$		
$t_0$	0.9682	0.9682	0.9682	0.9682	0.9682		
$t_1$	$0.2876 \times 10^{-2}$	$0.2874 \times 10^{-2}$	$0.2874 \times 10^{-2}$	$0.2874 \times 10^{-2}$	$0.2874 \times 10^{-2}$		
PC	1.0001	1.0001	1.0002	1.0003	1.0004		

Table 7 Same as Table 6, but for  $\theta_0 = 49^\circ$ . Results for Case II alone are presented

(Tables 6 and 7). These results show that the differential method becomes computationally unstable.

Finally, in Fig. 2, we show plots of the reflection and refraction efficiencies as functions of the angle of incidence for Cases I and II, when h/d = 0.05 and for p-polarized incidence. Although the efficiencies for Cases I and II are identical in the absence of corrugations, the efficiency curves are different when the boundary is corrugated, as can be appreciated from the figure.



Fig. 2. Reflection and refraction efficiencies for a sinusoidal grating with h/d = 0.05 illuminated from the vacuous side by a p-polarized plane wave, when  $\lambda_0 = 1.5d$  and  $\theta_c = 60^\circ$ . The constitutive scalars of the diffracting medium are  $\epsilon_{\perp} = -2.1$ ,  $\epsilon_{\parallel} = 1.9$ ,  $\mu_{\perp} = 1.3$  and  $\mu_{\parallel} = -1.6$  (Case I) or  $\epsilon_{\perp} = 2.1$ ,  $\epsilon_{\parallel} = -1.9$ ,  $\mu_{\perp} = -1.3$  and  $\mu_{\parallel} = 1.6$  (Case II). (a)  $r_0$ ; (b)  $t_0$ ; (c)  $t_{-1}$ .

# 6. Concluding remarks

From our studies, we concluded that the application of the differential method can also lead to non-convergent results for gratings made of materials characterized by indefinite constitutive tensors. The lack of convergence can be attributed to the existence of an infinite number of propagating harmonics refracted into the grating medium – a feature that, in principle, would limit the applicability of all theoretical methods commonly used nowadays for gratings. Expecting that the application of a general computational technique, such as the finite-difference-time-domain method [19], may be more successful than of specialized grating methods, we have commenced the next phase of our research in this emerging area.

### Acknowledgments

R.A.D. and M.E.I. acknowledge financial support from Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Agencia Nacional de Promoción Científica y Tecnológica (ANPCYT-BID 1201/OC-AR-PICT14099) and Universidad de Buenos Aires. A.L. is grateful for financial support from the Penn State CIRTL Project funded by the US National Science Foundation.

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