Analysis of dielectric gratings of arbitrary profiles and thicknesses: comment

M. Nevière

Laboratoire d'Optique Electromagnétique, Unité de Recherche Associée au Centre National de la Recherche Scientifique no. 843, Faculté des Sciences et Techniques de St-Jérôme, Avenue Escadrille Normandie-Niemen, 13397 Marseille Cedex 13, France

E. Popov

Institute of Solid State Physics, Bulgarian Academy of Sciences, Boulevard Trakia 72, Sofia 1784, Bulgaria

Received January 3, 1992; revised manuscript received April 21, 1992; accepted April 28, 1992

To reveal the advantages and capabilities of a recently published method [J. Opt. Soc. Am. A **8**, 755 (1991)] for the improvement of the modal approach to the analysis of gratings, we propose some additional numerical experiments in cases in which the previous differential method is known to fail.

In a recent paper[1] Pai and Awada proposed a method of computing the efficiencies of deep dielectric gratings in TE-polarized light (electric-field vector parallel to the grooves). The authors of Ref. 1 claim that their method is numerically stable, whatever the groove depth of the grating may be. Starting from the propagation equation of the field in the region of the modulated refractive index (which equation is the basis of the differential approach[2,3]), they discretize the y variable of integration (perpendicular to the grating plane) into several layers. Inside each layer the refractive index is assumed to be independent of the y axis, and the solution within each layer can be expressed in terms of eigenmodes, as has usually been done (see Refs. 19–31 of Ref. 1). The novelty of the method proposed by Pai and Awada lies in the following step, which is necessary for the final solution: the sewing together of the different modes (eigenfields) in the separated layers. Pai and Awada introduce layer transmission matrices and interface reflection and transmission matrices, and, in terms of these matrices, they derive the solution in terms of a multiple-reflection series that seems stable with respect to the usual numerical difficulties associated with the undesired exponential functions of the evanescent field components. They claimed their method to be stable, whatever the groove depth.

To prove their assertion, Pai and Awada[1] gave two numerical examples with different modulation depths. First the efficiencies of gratings with classical groove shapes (sinusoidal, triangular, and lamellar) are calculated for a groove depth-to-period ratio h/d equal to 0.67 and a wavelength-to-period ratio $\lambda/d = 1.67$. The grating material is assumed to be a dielectric with a refractive index equal to $\sqrt{3}$ or to 2. Second, Pai and Awada present numerical results for a very deep ($h/d = 4$) lamellar grating with $\lambda/d = 1$.

To verify their results (and, more importantly, the capacities of this new approach), we made calculations of the same examples with two different numerical methods: the codes based on the original differential formalism[2] and on the classical modal method[4] applied to the lamellar gratings. In the first case ($h/d = 0.67$) we found exactly the same results by using the classical differential method, as in Figs. 6, 8, and 9 of Ref. 1. But in the second case ($h/d = 4$) the original differential method failed to give convergent results, owing to the growing exponential factors of evanescent fields. On the other hand, the use of the classical modal method results in exactly the same data as those presented in Fig. 7 of Ref. 1. We decided not to give the corresponding curves in this Communication, since they are not noticeably different from those of Ref. 1.

The conclusion is that the method proposed in Ref. 1 is a nice improvement over the differential method, since it succeeds for modulation depths for which the original differential method fails, and it can deal with profiles out of the reach of the classical modal method. With the development of binary optics, the problems of deep gratings concern many scientists; thus it is desirable to have a more accurate idea of the exact capacities of this new method.[1]

The aim of this Communication is to draw the attention of grating investigators and, in particular, of the authors of Ref. 1, to some conditions useful for further numerical experiments, to determine the capabilities and limits (which surely exist) of the method. These conditions are quite natural and pertain directly to the essence of the method. Moreover, the conditions concern not only this specific improvement of the differential method but all numerical methods for light diffraction by relief gratings:

1. The numerical results presented in Ref. 1 pertain to conditions under which only one or two orders propagate, since λ/d is taken to be 1.67 or 1. This condition underlies the reason why a triangular grating could be successfully approximated by few (six or even two) steps (see Fig. 10 of Ref. 1); it is well known from the famous equivalence rule[5] that, if a grating supports only two diffraction orders, the exact grating profile is of little significance, since the predominant role is played by the first Fourier

0740-3232/92/112095-02$05.00

component of the profile. Unfortunately it does not hold for other cases of shorter wavelengths. Thus it would be useful and interesting to have more numerical results covering the shorter-wavelength region (say, $1 > \lambda/d > 0.3$), where more propagating orders exist. In these cases not only is profile-form discretization important, but more vertical slides are needed owing to the increase in the h/λ ratio. Information concerning the lowest λ/d ratio beyond which computation difficulties arise, as well as some examples of the necessary computation time, is desirable.

2. Most sensitive to the capability and the efficiency of the different numerical methods is the numerical modeling of light diffraction by metallic gratings. Even for commercial gratings ($h/d < 0.4$) difficulties often arise even for nonsmall λ/d ratios. For example, one of the principal difficulties in the modal method, which would also exist for the proposed method in Ref. 1, is the complexity of the eigenvalues in the case of lossy materials as well the nonorthogonality (and probably noncompleteness) of the set of eigenvectors. Furthermore, owing to the growing exponentials, even in the TE case, the classical differential method is restricted to a modulation depth of ~ 0.8 in the case of highly reflecting materials. Thus it is important to know the capabilities of the novel method with respect to metallic gratings, in view of the fact that the method does not seem to suffer from the problem of exponentials. We cannot stress enough how important this can be from the practical point of view.

3. In the case of TM polarization (electric-field vector perpendicular to the grooves) the difficulties of the classical differential method increase rapidly with the reflectivity of the grating material even for the most common cases of $h/d \in (0.1, 0.4)$. Contrary to the TE case, the numerical problems arise now mainly because of the slow convergence rate (to the power of -1) of the Fourier series used to describe the electromagnetic field. In our laboratory, we have already succeeded in getting rid of the nonorthogonality difficulty[6] mentioned above by deriving an improved differential method[7] that applies Schmidt orthonormalization of the functions in the course of integration. This enables us to deal with aluminum gratings in the visible region without any numerical instabilities, even for TM polarization up to a groove depth of $h/d = 0.2$ (see Ref. 6). We applied our improved differential method to the thick grating example of Fig. 7 in Ref. 1 and encountered no overflowing, even for a metallic substrate and TM polarization. But the main problem remains the slow rate of convergence of the Fourier series, in which, even with 101 Fourier components, our result is still more than 7% away from those of the integral method. We have the notion that this problem would also exist in the method of Ref. 1.

In any event, the new improvement of the differential method proposed by Pai and Awada[1] seems powerful for the investigation of deep dielectric gratings. The method would be even more useful if it proves to work well enough for small λ/d ratios, metallic gratings, and TM polarization.

E. Popov recently held a postdoctoral position at the Laboratoire d'Optique Electromagnétique, Marseille.

REFERENCES

1. D. M. Pai and K. A. Awada, "Analysis of dielectric gratings of arbitrary profiles and thicknesses," J. Opt. Soc. Am. A **8**, 755–762 (1991).
2. M. Nevière, P. Vincent, and R. Petit, "Sur la théorie du réseau conducteaur et ses applications à l'optique," Nouv. Rev. Opt. **8**, 65–77 (1974).
3. P. Vincent, "Differential method," in *Electromagnetic Theory of Gratings,* R. Petit, ed., Vol. 22 of Topics in Current Physics (Springer-Verlag, Berlin, 1980), p. 101.
4. I.C. Botten, M.S. Craig, R.C. McPhedran, J.L. Adams, and J.R. Andrewartha, "The dielectric lamellar diffraction grating," Opt. Acta **28**, 413–428 (1981).
5. See, for example, D. Maystre, M. Nevière, and R. Petit, "Experimental verifications and applications of the theory," in *Electromagnetic Theory of Gratings,* R. Petit, ed., Vol. 22 of Topics in Current Physics (Springer-Verlag, Berlin, 1980), p. 181.
6. M. Nevière and P. Vincent, "Differential theory of gratings: answer to an objection on its validity for TM polarization," J. Opt. Soc. Am. A **5**, 1522–1524 (1988).
7. G. Tayeb, Laboratoire d'Optique Electromagnétique, Faculté des Sciences et Techniques de Saint-Jérôme, Marseille, France (personal communication, 1986).