Grating Electromagnetic Theory User Guide

M. Nevière and E. Popov†

Laboratoire d'Optique Electromagnétique, case 262, Faculté des Sciences et Techniques de Saint Jérôme, Av. Escadrille Normandie- Niemen, 13397 Marseille Cedex 20, France

Recent state-of-art applications of diffraction gratings and stratified materials with one or several modulated interfaces impose specific requirements on electromagnetic grating theory. A review of such applications is presented here with an emphasis on the aspects of the theoretical methods required for their efficiency prediction and optimization. A brief review of the basic ideas of the various electromagnetic theories used is given. The specific domain of validity for each theory is discussed together with advantages and shortcomings. The aim is to serve as a guide in selecting the most appropriate theoretical method for handling specific grating problems.

Journal of Imaging Science and Technology 41: 315–323 (1997)

Introduction

Two centuries after the discovery of gratings by Rittenhouse,[1] gratings and more complicated periodic structures have become common not only in spectroscopy but also in numerous domains of physics such as acoustics, solid state physics, nonlinear optics, x-ray instrumentation, optical communications, and information processing. Moreover, gratings began to appear in common use in CD players, as safety features on credit cards and bank notes, as well as in variety of display and advertising applications.

The term grating is no longer restricted to periodically modulated surfaces and is also used for modulated devices with varying periods, curved grooves, or varying groove shapes, such as Fresnel planar lenses and diffractive optic elements. Such structures are used in integrated optics to achieve beam focusing and beam shaping. Their diffraction properties can still be related to the corresponding gratings, as far as an adiabatic variation of the groove geometry can be assumed, i.e., the groove change is carried out over a large number of grating periods.

The following section reviews the various types of gratings, quasi-gratings, and periodically modulated stratified media in use in various domains of science. The next section presents a brief description of the most commonly used theoretical diffraction methods. The final section before the conclusion provides a user guide to grating theories devoted to helping scientists select the method most suitable for a given particular problem.

Review of the Grating Problems

The classical grating problem consists of a bare metallic grating used in reflection for spectroscopic purposes. Figure 1 represents a triangular groove grating usually called an *echelette* grating and defines some notations to be used further. Such gratings are usually produced by diamond ruling. Holographic recording, beam-etching and lithographic methods produce, in general, symmetrical profiles with sinusoidal, lamellar (rectangular), or trapezoidal grooves. Electron microscopy reveals that for very high groove frequencies (e.g., 6000 groove/mm), as well as very low ones (e.g., echelles, widely used in astronomy), the real profiles have much more complicated form, different from the classical four types mentioned below.

In far-infrared and millimeter range of wavelengths, the metal can be assumed to have infinite conductivity. In the visible region and for shorter wavelengths, the finite conductivity complicates the grating response and requires different theoretical methods.

Transmission gratings are frequently used as beam splitters and as *grisms* (Fig. 2) to transform a telescope or a camera into a spectroscope. Under special conditions the diffraction compensates the refraction and a dispersive diffraction order can propagate in the initial direction, Fig. 2. Transmission gratings require a transparent (lossless) grating material, in contrast to reflection gratings.

Grating couplers combine a dielectric grating and an optical waveguide (Fig. 3). They are used in integrated optics to couple an incident beam into the slab or vice versa.

Dielectric coated gratings are mainly used in vacuum UV with a dielectric layer (typically MgF_2) to prevent

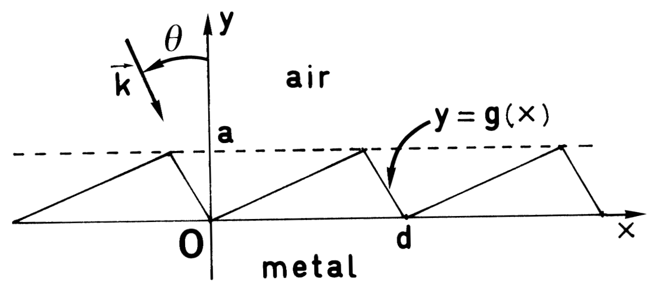

Figure 1. Schematic representation of a bare metallic grating. k is the incident wave vector.

Original manuscript received November 10, 1996.

† on leave from the Institute of Solid State Physics, Bulgarian Academy of Sciences, 72, Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

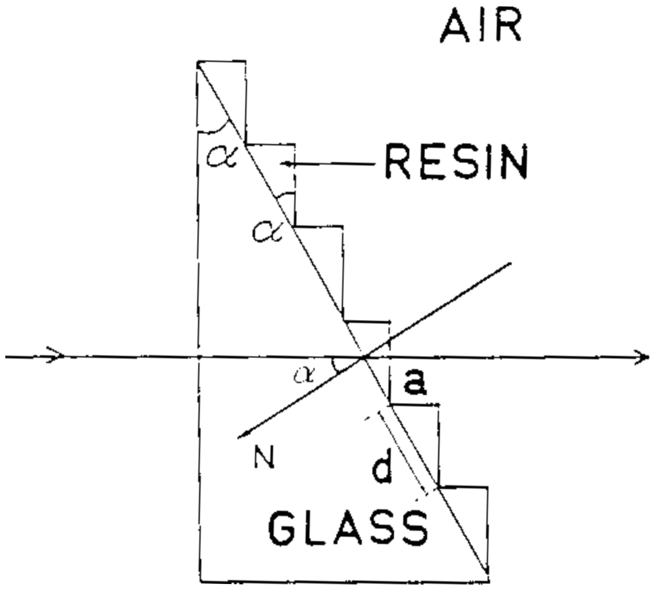

Figure 2. Schematic representation of a grism.

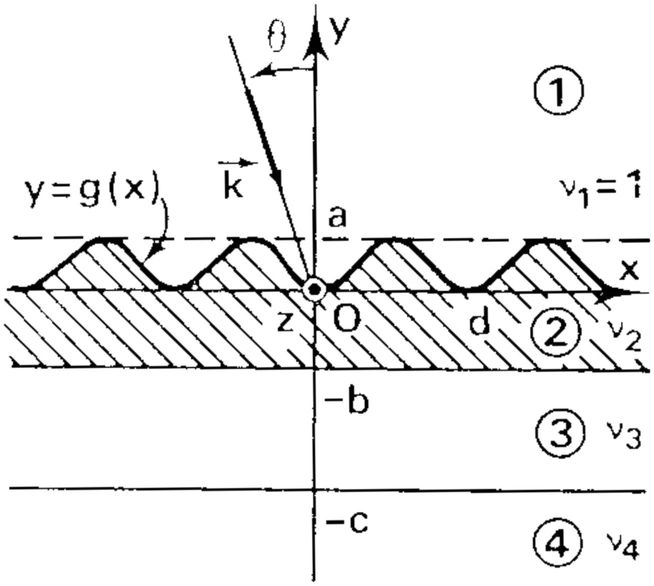

Figure 3. A grating coupler.

aluminum from oxidation (Fig. 4). A similar technique is used in the visible region to protect silver gratings from tarnishing.

Multilayer dielectric gratings consist of a dielectric grating replicated on the top or at the bottom of a stack of plane dielectric layers with alternating high and low refractive indices and a quarter of wavelength thickness (Fig. 5). They are used in high-power laser optics to achieve peak absolute efficiency, typically more than 96%, at a single wavelength.

Another kind of multilayer grating, consisting of a stack of modulated interfaces, is used in the XUV and x-ray domains. Their theoretical treatment requires us to distinguish between the two main cases: profiles without and with an interpenetration. No interpenetration occurs when the bottom of the upper profile lies higher than the top of the lower profile. A grating coupler with double corruga-

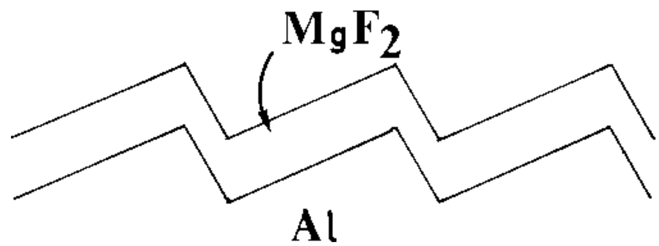

Figure 4. Dielectric coated grating for VUV region.

tion (Fig. 6) is an example of a thin stack of identical profiles without interpenetration. It can be optimized to couple as high as 80% of the incident beam into the waveguide. In a more complicated case (Fig. 7), the high diffraction efficiency (45%) in the XUV region (wavelength $\lambda \sim 15$ nm) is obtained by combining profiles with interpenetration (e.g., 2 and 3) and without (e.g., 1 and 2). The case of identical profiles is called a multilayer coated grating, and the layers are usually thinner than the profile depth, i.e., interpenetration occurs (Fig. 8). Such gratings are used in the two extremities of the spectrum. Another alternative high efficient grating for x-ray is the Bragg–Fresnel multilayer grating, as shown in Fig. 9.

Echelles are echelette gratings used in high orders, typically 10 to 500. They can be bare (Fig. 1) or multilayer coated (Fig. 8) depending on the spectral domain. The low wavelength-to-period λ/d ratio requires special theoretical methods.

The multilevel gratings used in diffractive optics to produce multiple beams from a single incident ray are illustrated in Fig. 10. Usually they also work with extremely low λ/d ratios.

In comparison, Dammann gratings, as illustrated in Fig. 11, consist of several bumps of different width within a single period. Not only do they also work in a low λ/d region, but in addition their profile is more complicated to introduce in grating theories. Dammann gratings have also become a common element in diffractive optics.

Gratings with varying period or groove shape are used in integrated optics and in the x-ray domain for focusing and beam shaping. If only the groove period is varied, we obtain a linear zone plate. When etched inside a planar multilayer structure, it is called a Bragg–Fresnel linear zone plate (Fig. 12), used in x-ray microscopy and spectroscopy.

Some gratings have discontinuous profiles, e.g., grid or rod gratings made of dielectric or metallic rods. The latter are used as frequency filters in infrared, selective absorbers of solar energy, or radar furtivity. In photolithography, chromium masks are made of rectangular rods (strips, sometimes called Ronchi gratings) and are used to cast their shadow onto a photoresist layer, which represents a combination of a rod grating and several plane layers.

Phase or volume gratings do not contain corrugated interfaces, but rather a plane layer with a periodic modulation of the refractive index. The result is that lamellar and rectangular rod gratings belong to both relief and phase grating types.

The next complications appears when going to two-dimensional geometry with a modulation of the index or corrugation of the surface made in two directions. The result is called a crossed grating, as illustrated in Fig. 13. Such devices can be useful in solar absorption, beam splitting, and memory storage. Their other name, bi-grating is often confused with a one-dimensional grating having two different periods of modulation.

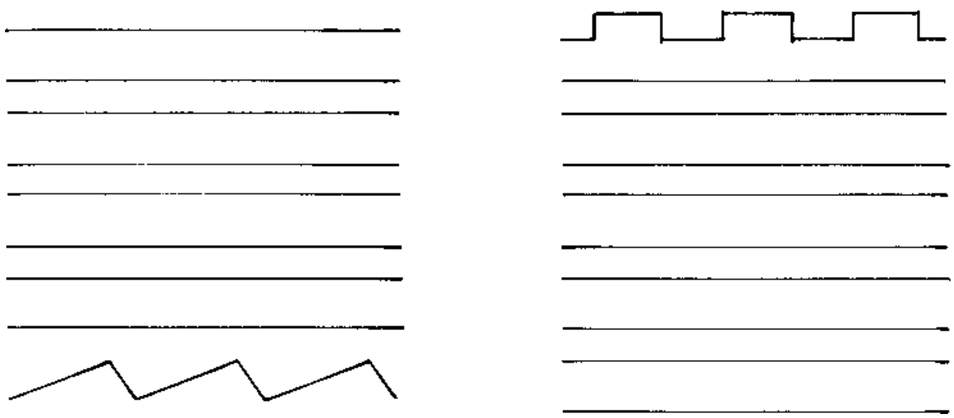

Figure 5. Two examples of multilayer dielectric diffraction gratings.

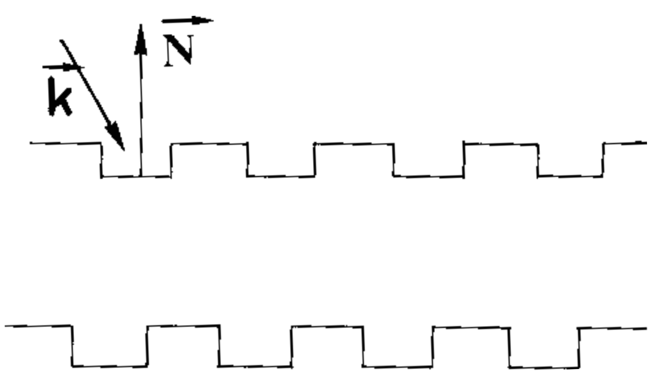

Figure 6. Grating coupler with double surface corrugation.

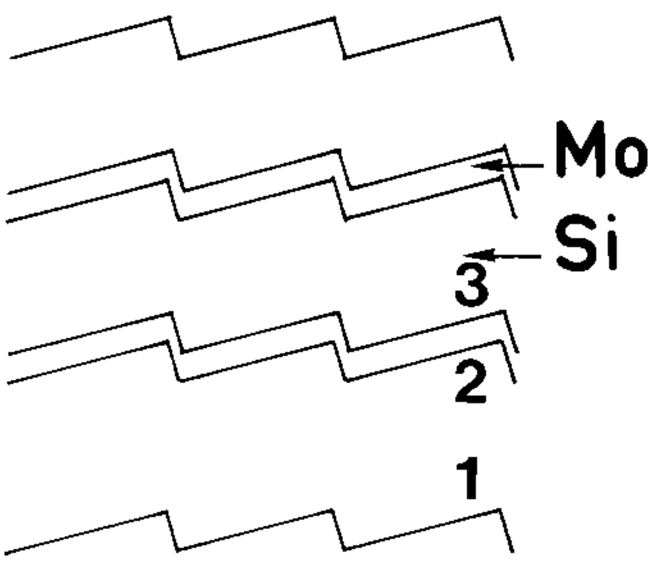

Figure 7. Stack of gratings for the XUV region.

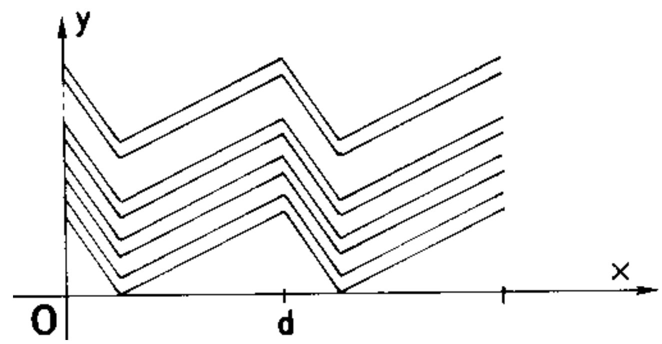

Figure 8. Multilayer coated grating.

Another problem that can be treated numerically using grating theories comes from the necessity to interpret the images of the photon scanning tunelling microscope. When a grating surface is studied, it is necessary to analyze the near-field picture as diffracted by a periodic surface in presence of a single object, namely the tip of the scanning device (optical fiber). This structure can be modelled by substituting the single tip with a collection of periodic tips with a distance much larger than the grating period to avoid parasitic coupling. The geometry is then reduced to two gratings with different periods, one being a multiple of the other.

In addition to geometrical complexity, the gratings can be made of anistropic, biaxial, or chiral material. Also they can be used in nonlinear optics for second harmonic generation, Kerr effect, and optical bistability, etc. This points out how complex grating problems may become. The next section will explain how to tackle them.

Basic Principles of Rigorous Electromagnetic Theories

Until recently grating properties were taught in universities in the frame of scalar optics. Grating were assumed to be a periodic collection of slits or small mirrors, and their diffraction phenomenon was analyzed with the Kirchhoff diffraction theory[2] in the Fraunhofer approximation. The Fraunhofer equation, which determines the direction of diffracted orders, was established and the dispersive properties of gratings were taught. But little was said about the distribution of energy among the various propagating orders. The normalized intensity was found to be a product of the normalized interference function and the normalized intensity function I_0 of a single slit. The intensity function falls off its maximum slowly in comparison with the interference function. Thus the intensity diffracted by the grating was found to consist of sharp peaks (due to the interference function), modulated by I_0,

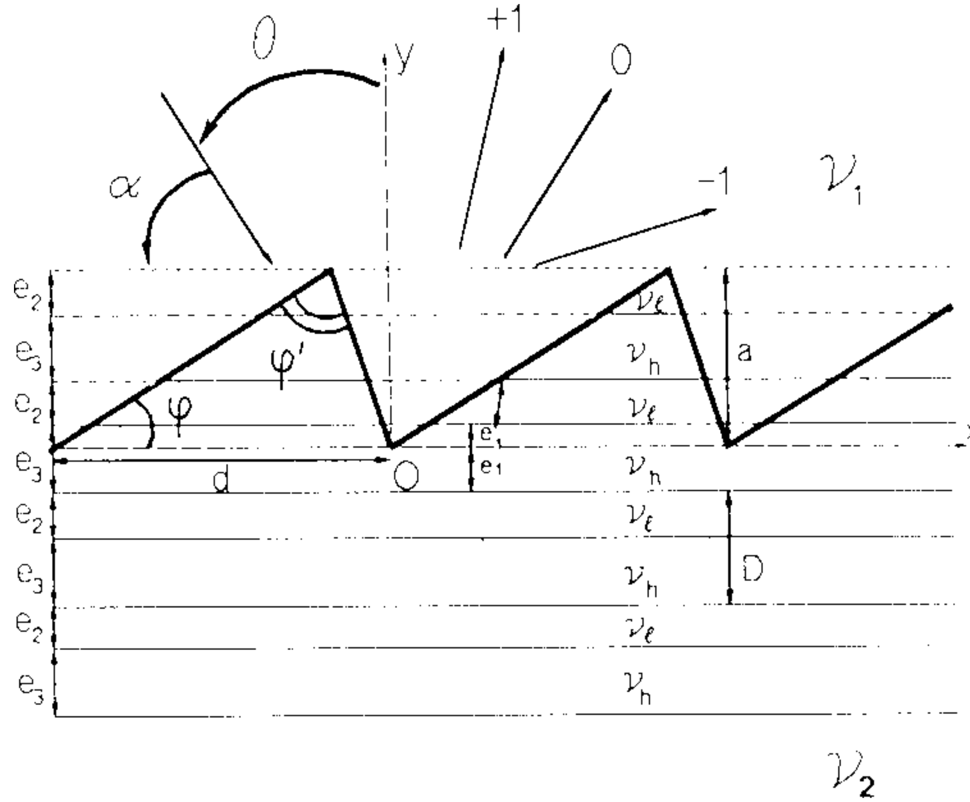

Figure 9. Bragg–Fresnel grating; ν_l and ν_h are the refractive indices of the low and high index layers, which have thicknesses e_2 and e_3, respectively, and D is the period of the multilayer ($D = e_2 + e_3$).

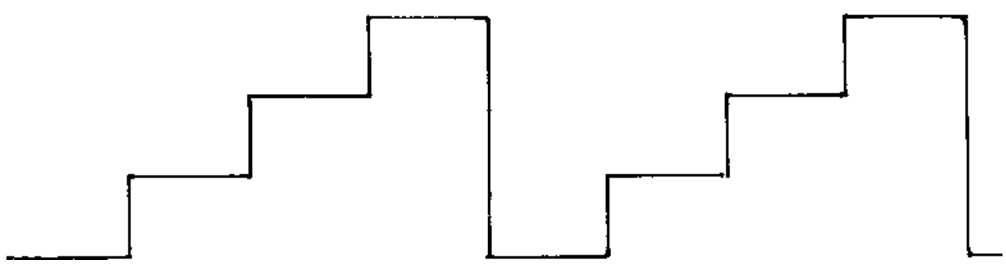

Figure 10. Multilevel grating.

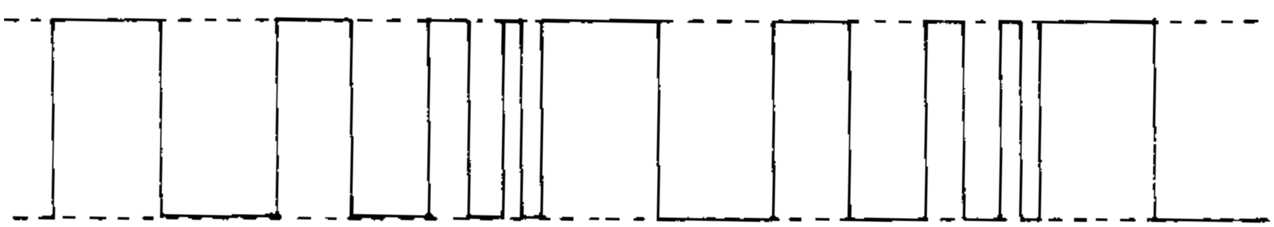

Figure 11. Dammanan grating.

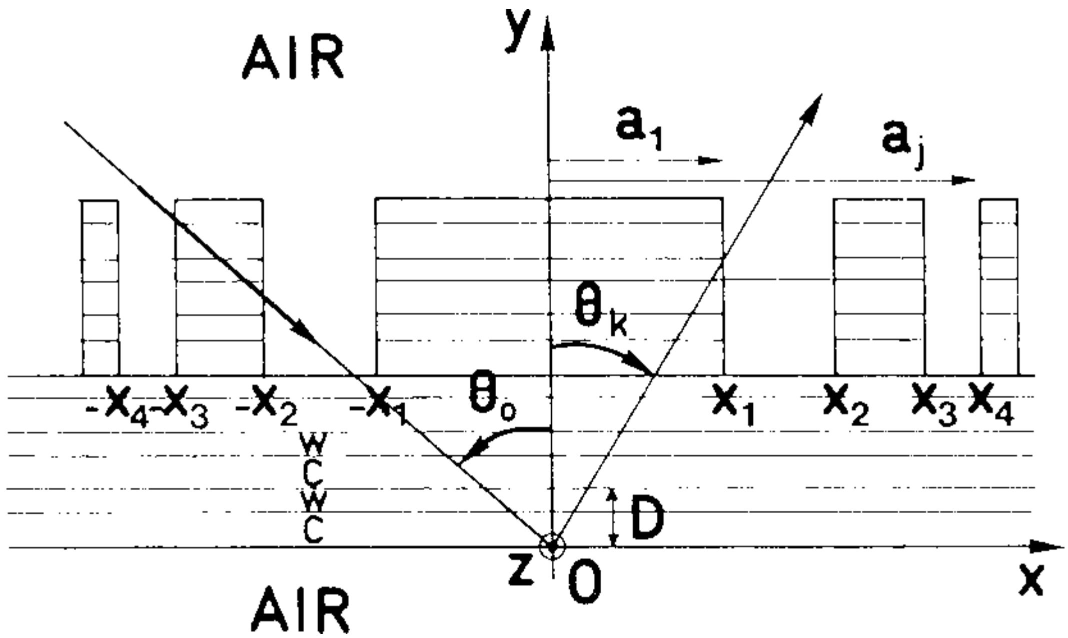

Figure 12. Bragg–Fresnel linear zone plate. The abscissae *xn* are equal to $x_n = \sqrt{n}a$, where $a = \sqrt{F\lambda} \,/\cos\theta_0$ (*F* is the focal length and λ the wavelength).

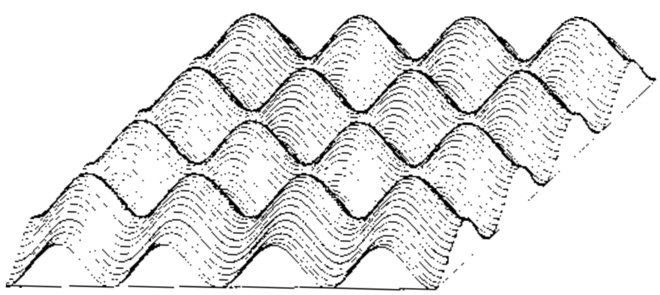

Figure 13. Crossed grating.

which depends on the groove shape (slit, mirror, etc.). While such an approach can predict that 100% of the incident energy can be concentrated inside one order,[3] it is not capable of fully taking into account the polarization effects, neither can it account for the existence of Wood anomalies. Although improved by several authors[4,5], such an approach fails in the resonance domain where λ/d ratio is close to unity, typically lying between 0.2 and 5. The approach can be used only in the short wavelength regime, and even there can be erroneous under high incident angles. However, the scalar approach is capable of bringing some physical insight and making good predictions for near normal incidence. Because the approach is not reliable in general, we concentrate here on electromagnetic theories, starting with the simplest.

The Rayleigh Theory[6]. Let us consider the grating illustrated in Fig. 1 with an incident plane wave having an electric field vector parallel to Oz axis (TE, *P*, or *s* polarization). The *z*-component of the electric field can be written as:

$$E^i(x,y) = A\exp\left[ik(x\sin\theta - y\cos\theta)\right],$$

assuming $\exp(-i\omega t)$ time dependence. Such function obviously satisfies a pseudo-periodicity property:

$$E^i(x+d,y) = E^i(x,y)\exp(i\gamma d),$$

with $\gamma = k \sin\theta$. The Floquet theorem requires that the total field $E(x,y)$ is quasi-periodical, thus $E(x,y)\exp(-i\gamma d)$ can be expanded into Fourier series, i.e.,

$$E(x,y) = \sum_{n=-\infty}^{\infty} E_n(y)\exp(i\gamma_n x) \tag{1}$$

with

$$\gamma_n = \gamma + nK$$
$$K = \frac{2\pi}{d}.$$

In each homogeneous region defined by $y \notin [0,a]$, Maxwell equations lead to a Helmholtz equation:

$$\Delta E(x,y) + k_0^2\nu^2 E(x,y) = 0 \tag{2}$$

where ν is the refractive index of the medium, $k_0 = \omega/c$, and *c* is the light velocity. Substitution of Eq. 1 into Eq. 2 leads to an analytical expression for $E_n(y)$:

$$E(x,y) = A\exp\left[i(\gamma_0 x - \beta_0 y)\right] + \sum_{n=-\infty}^{\infty} B_n \exp\left[i(\gamma_n x + \beta_n y)\right] \tag{3}$$

with

$$\beta_n^2 = k_0^2\nu^2 - \gamma_n^2.$$

In metals, the corresponding expression includes the metal complex refractive index, unless the metal is perfectly conducting. Expression (3) is called Rayleigh expansion. The Rayleigh method[6] assumes that Eq. 3 is valid not only outside the modulated region but also inside the grooves. This enables one to explicitely write the boundary conditions, but this hypothesis has been shown to be not valid in general. A detailed discussion can be found in Ref. 7. In particular, the Rayleigh method is valid for sinusoidal perfectly conducting gratings when the groove depth-to-period ratio does not exceed 0.142. Outside this domain, however, sometimes the method gives acceptable results for the far field, while the errors in the near field are greater.

Although never valid theoretically for profiles with edges, the method can be used succesfully at low blaze angles for triangular grooves and for low groove depths for lamellar gratings. In addition, the variational formulation of the Rayleigh hypothesis known as the Yasuura method[8] is rigorous whatever the groove shape may be.

Differential Theory.[9a,b] Instead of using two analytical expressions of $E(x,y)$ and matching them on the grating profile, the differential theory distinguishes between the homogeneous regions ($y \notin [0,a]$) where Rayleigh expansion such as Eq. 3, are valid and a modulated region ($0 < y < a$) where a numerical integration is carried out. In the modulated region, the Helmholtz equation is changed into:

$$\Delta E(x,y) + k_0^2 \varepsilon(x,y) E(x,y) = 0. \tag{4}$$

Introducing Eq. 1 into Eq. 4 leads to a system of ordinary differential equations with nonconstant coefficients of the form:

$$\boldsymbol{E}''(y) = \boldsymbol{V}(y)\boldsymbol{E}(y), \tag{5}$$

where $\mathbf{E(y)}$ is a column vector with components $E_n(y)$ and $\mathbf{V(y)}$ is a square matrix whose elements depend on the Fourier components $\varepsilon_m(y)$ of the permittivity:

$$V_{mn}(y) = \varepsilon_{m-n}(y) - \gamma_n^2 \delta_{mn}.$$

A numerical integration of Eq. 5 is performed using a standard algorithm. Matching the numerical solution with the Rayleigh expansions at the boundaries of the modulated region ($y = 0$ and $y = a$) enables us to find the Rayleigh coefficients (B_n in Eq. 3) and thus the field everywhere.

Numerical instabilities from growing exponential functions during the integration may appear when dealing with deep gratings or stacks of interpenetrating gratings. Recent developments[10] gathered under the names of **R**-matrix and **S**-matrix propagation algorithms eliminate this difficulty. The **S**-matrix algorithm is easier for use.[10,11] Similar difficulties can arise when a low-modulation grating is combined with a thick stack of plane layers. The problems are solved using similar methods: the **S**-matrix algorithm or the impedance method.[12] The only numerical problem that remains is linked with the truncation of the set in Eq. 5 required for numerical implementation of the theory. It assumes that the field is correctly described by a limited ($2N + 1$) number of Fourier components in Eq. 3. Obviously, the number N will be different if the field and its normal derivative are continous across the grating surface, as it is in the TE case of polarization, or strongly discontinuous, as happens for the normal derivative for metallic gratings in TM polarization. Numerical experience shows that the truncation parameter N can vary between 4 and 100, depending on the polarization, groove depth, and grating material. Because computation time is roughly proportional to N^3, it can vary by a factor of 15,000 depending on the problem. Small N leads to very short computation times, less than a second on most of the small workstations.

Note that for perfectly conducting metals, the modulus of the permittivity increases infinitely and Eq. 2 cannot be used. Conformal mapping[13] is used then to transform the grating surface into a plane, making the corrugated surface equivalent to a phase grating on a plane surface, which latter problem can be easily resolved by the differential theory.

Method of Moharam and Gaylord.[14a,b] For lamellar (rectangular, laminar) profiles, the function $\varepsilon(x,y)$ does not depend on the vertical coordinate y and a solution of Eq. 5, or its equivalent for TM polarization, can be found without numerical integration using the eigenvalue/eigenvector technique. The field in the modulated region is represented as a superposition of modes in the form

$$c_m \exp\left(i\sqrt{\xi_m}\, y\right),$$

where ξ_m are the eigenvalues of matrix $\mathbf{V}$. The unknown coefficients c_m are determined from the boundary conditions at the limits of the modulated region ($y = 0$ and $y = a$). This method was originally called the modal method and nowadays is known as rigorous coupled wave theory. The theory uses the same differential equations and basic functions as the differential theory. The difference is in the numerical method, specific to the lamellar profile. Because each profile can be more or less precisely represented in a staircase approximation, the method of Moharam and Gaylord has been generalized to arbitrary profiles. It then appears to be quite similar to the classical differential theory. While in differential theory the discretization of $\varepsilon(x,y)$ is made during the numerical integration, the Moharam and Gaylord method makes the discretization by substituting the real profile with a staircase function. Thus problems due to numerical instabilities are quite similar in both methods, as are the approaches for their resolution.

Classical Modal Method.[15a,b] For a steplike (lamellar, rectangular) profile, use of the Fourier series expansion 1 is not even necessary with respect to the x axis. A solution of the Maxwell's equations can be found in closed form in each of the grooves and lamellae in Cartesian coordinates:

$$F_m(x,y) = u_m(x) e^{i\mu_m y}, \tag{6}$$

so that the function $u(x)$ has a different form inside the grooves and inside the lamellae, determined by the optical index of the media. The boundary conditions are then applied on the vertical groove walls. Owing to periodicity, a discrete set of values exist for μ, called modal constants. The total field is then represented as a sum over all the modes of the corrugated system, and the coefficients in the modal expansion are determined from the boundary conditions on the interfaces between the corrugated and the homogeneous media. Unfortunately, for highly conducting materials (again!), the modal constants are spread over the complex plane and cannot be easily located. Several different techniques have been proposed.[16a,b]

The main disadvantage of the modal method is that it is too narrowly specialized and can be applied to profiles other than the lamellar one only if represented as a few rectangular steps. Recently an interesting generalization to arbitrary profiles has been proposed.[17] The main advantage is that each of the modes represents a solution of Maxwell's equation and the boundary conditions inside the different media of the corrugated region, so evaluation of the electromagnetic field characteristics inside the grooves becomes possible with great precision. The main difference in comparison to the classical differential method and the method of Moharam and Gaylord is that the classical model method does not require a Fourier representation of permittivity and the field components at both sides of the corrugated interface and so can easily deal with highly reflecting surfaces.

Integral Theory.[18a,b] The integral method was the first rigorous grating theory. The method was developed by several authors in circa 1966 for perfectly conducting gratings and generalized in 1972 for finite conductivity.[18a,b] The basic principle of the integral method can be understood more easily for perfectly conducting substrates. When an incident plane wave falls on the grating surface, the wave induces a surface current $j_S(M')$ at each point M' of the surface. When propagating along the grating, the surface current radiates a diffracted field $E(P)$ at a given point P above the surface. Provided j_S is known, $E(P)$ can be found through the Kirchhoff-Huygens formula using the Green function technique, so that:

$$E(P) = \int_{\substack{\text{one grating}\\ \text{period}}} G(P,M')\varphi(M')ds', \tag{7}$$

where $\varphi(M')$ is proportional to $j_S(M')$, $G(P,M')$ is the Green function, which is known, and the integration is carried over the curvilinear coordinate s' along the grating profile.

However, the problem is more complex than just a single integration, because the surface current is not produced only by the incident wave, but results also from the diffracted field radiated from the other points of the grating. Thus $j_S(M')$ depends both on E^i and on the values of the current $j_S(M'')$ at each other point M'' of the profile, different from M'. This is why Eq. 7 is transformed into an integral equation for $\varphi(M')$. The situation becomes even more complicated for finitely conducting gratings.[18a,b] The key point of the theory is the numerical resolution of an integral equation with a singular kernel. Fortunately, the singularities can be eliminated analytically, and then the integral equation is transformed into a linear set of algebraic equations by discretization along the grating profile.

The greatest advantage of the integral formalism, when compared to the differential method, is that it "follows" the profile, without crossing it. As a result, it is not necessary to develop into Fourier series some quantities that exhibit a jump over the surface. Sometimes, however, this can be a disadvantage, as in the case of nonlinear dielectrics, characterized by volume distributed sources, which are difficult to include in the integral equation. In addition, working in real space, instead of the transformed one, requires numerical derivatives, if all the field components are searched near the surface.

As a result of its generality, the integral theory is able to deal with practically any kind of grating, including some limiting cases where it is the only available method. Examples here are echelle gratings (used in 50, 100, or even higher orders and at high angles of incidence) and highly conducting very deep gratings with arbitrary profiles, etc. This advantage is obtained at the cost of more complex mathematics, larger codes, and longer computation times, as well as larger memory storage requirements. The complexity of the theory also makes more difficult its adaptation to phase gratings, anisotropic media, profiles with interpenetration, etc.

Method of Coordinate Transformation.[19a,b] An effort to combine the relative simplicity of the differential theory with the advantage of the integral theory of not crossing the profile results in another approach,[19a] based on a coordinate transformation

$$Y = y - g(x) \tag{8}$$

that transforms the grating surface $[y = g(x)]$ into a plane Y = constant. Maxwell equations can be integrated at each side of this plane separately and the solutions then matched along the surface. Although the transformation is curvilinear and nonorthogonal, fortunately it is possible to reduce Maxwell equations to a set of ordinary differential equations with constant coefficients, which can be written in a matrix form:

$$\frac{d\mathbf{F}}{d\mathrm{Y}} = \mathbf{TF}(\mathrm{Y}) \tag{9}$$

Because matrix $\mathbf{T}$ is independent of $\mathbf{Y}$ the solution of Eq. 9 can be expressed in terms of eigenvalues ρ_m and eigenvectors C_{mn} of $\mathbf{T}$:

$$F_m = \sum_n C_{mn} e^{i\rho_n Y} b_n. \tag{10}$$

After that, the expansions Eq. 10 above and below the corrugation are matched on the flat boundary Y = const, taking into account the appropriate outgoing wave conditions. The diffraction order amplitudes can be obtained by backward transformation of the basis Eq. 10 after the amplitudes of the field expansion are determined. Because this method does not require crossing the profile during a search for the solution, but only when matching the different expansions, it is able to deal with deep gratings independent of polarization and refractive index, and including multilayer gratings. The method has relatively simple computer codes and short computation times comparable to those of the differential method. The ease of incorporating several overcoating layers that follow the initial profile may be stressed. The main limitation concerns the types of profile with which the method can deal. This limitation comes from the nature of the coordinate transformation 8, that does not allow noncontinuous functions $g(x)$. Strictly speaking, the method requires the derivative of $g(x)$ be a continuous function, so edges are excluded, but this is true of all the electromagnetic methods and, fortunately, nature does not allow edges. In practice, the slope of the steepest part of the profile is much more important: when $g'(x)$ becomes large, not only does its Fourier representation slowly converge, but the transformation of the coordinate system degenerates. The derivative with respect to the first and second coordinates tend to each other

$$\left(\frac{\partial}{\partial x} \to \frac{\partial}{\partial Y}\right).$$

However, numerically this limitation is not so severe as appears: sinusoidal gratings with $h/d > 10$ have a very steep slope, but only along a limited part of the profile and can be successfully treated, while lamellar gratings are excluded by definition and triangular gratings with limited asymmetry of the profile can be treated without difficulties.

Other theoretical methods for grating diffraction do exist, like the conformal mapping technique for finite conductivity, the finite-element method, the fictitious sources

TABLE I. Ability (shown by Asterisks) of Grating Theories to Deal with Simple Gratings Problems

Methods	Perfectly conducting gratings	Dielectric gratings	Real metals	Deep dielectric gratings	Deep metallic gratings	Binary gratings	Dielectric coated gratings	Multilayer dielectric gratings	Low modulated gratings
Rayleigh	*	*	*				*	*	****
Differential		*****	***	*****	**	***	***	*****	*****
Moharam & Gaylord		****	**	****	***	****		****	****
Modal	***(*)	****	***(*)	****	***(*)	*****		****	****
Integral	*****	****	*****	*****	*****	**	****	****	****
Coordinate transform.	****	****	****	*****	*****		*****	***(*)	*****
Conformal mapping	****						***		

TABLE II. Ability (shown by Asterisks) of Grating Theories to Deal with Exotic Gratings Problems

											Nonlinear optics			
Methods	Bare metallic echelle	Bare dielectric echelle	Multilayer x-ray echelle	Phase gratings, holograms	Multilevel gratings	Dammann gratings	Multilayer coated gratings	Anisotropic, chiral, etc. media	Bragg–Fresnel gratings	Crossed gratings	SHG[1] in dielectrics	SHG in metals	Kerr effect	X-ray domain
Rayleigh								****		*	*			****(*)
Differential	**	*****	*****	*****	***	****	*****	*****	*****	***	****	***	*****	*****
Moharam & Gaylord				*****	*****	*****			****	**	***	**	****	****
Modal					****	*****		*	****	**	***	**	***	
Integral	*****	*****			*****	****	**	*	***	*****		*****	****	*
Coordinate transform.							*****	**		*****[2]	*****	****	****	****

[1] SHG = second harmonic generation
[2] the coordinate transformation suitable for these problems is consideredin Ref. 20.

method, etc., but we limit ourselves here to the methods that have proved themselves in tackling many grating problems and that have the corresponding computer codes in regular use.

Grating Theory User Guide

The diversity of grating problems and existing theories today is so great that it is not obvious for an engineer or a scientist which method is best suited to resolve the problem he encounters in his work. To try to help him in this aim, we first distinguish between two kinds of grating problems: The first kind are simple grating problems and concern relief gratings made with homogeneous isotropic materials that are used in linear optics in the resonance domain. The modulated region will be limited to one or a few (less than 3) nonseparable interfaces, plus a stack of plane interfaces and other separable modulated interfaces if any. The second kind are exotic situations and include bare echelles, multilevel and Dammann gratings ($\lambda/d <<$ 1), phase gratings, multilayer coated gratings and echelles, gratings ruled on anisotropic materials, gratings used in nonlinear optics, crossed gratings, Bragg–Fresnel gratings, and any kind of x-ray gratings.

Table I lists the relative merit of the theories used to confront the various types of simple grating problems. The criteria of simplicity, short computation time, and universality (groove shape, TE and TM polarization, etc.) are added to the performance of computation in view of attributing the number of asterisks for each method. The general impression is that if we except the low modulated case, a grating with high (but not infinite) conductivity will be analyzed through the integral theory or through the coordinate transformation method. For dielectric gratings, the differential theory is preferred. The same criteria are used to construct Table II, which gives an idea of the versatility and universality of the theories when confronted with new problems.

To illustrate how these tables can be used, let us go back to the grating problems described in the above section, **Review of Grating Problems**, and give our preferred theory for each problem. Keep in mind that in most cases several theories could work. The metallic grating in Fig. 1 would be studied with the integral method; the transmission gratings in Figs. 2 and 3 with the differential theory as well as the dielectric coated grating for VUV region, except if the groove depth is high, in which case we would go back to the integral method. The multilayer dielectric grating in Fig. 5 would be studied with the differential method, the lamellar grating coupler in Fig. 6 with the Moharam and Gaylord method. The stack of gratings in Figs. 7 and 8 as well as the Bragg–Fresnel gratings and zone plate in Figs. 9 and 12 would be studied with the differential method; the multilevel grating in Fig. 10, with the integral method; the Dammann grating in Fig. 11 with the differential theory, the crossed grating in Fig. 12 with coordinate transformation.[20] In addition, phase gratings and holograms would be studied with the differential technique and grid gratings with the differential or integral theory depending on whether the rods are dielectric or metallic. These examples give an idea of the choice that should be made for various problems encountered in linear optics.

Conclusion

The limitations, advantages, and potential of the most important grating theories have been discussed. No theory is actually universal in the sense that no computer code that should be able to analyze any grating problem still exist. But for most classical gratings problems, several methods are available. The aim of this paper is to guide scientists and engineers in their choice.

References

1. D. Rittenhouse, An optical problem proposed by F. Hopkinson and solved, *J. Am. Phil. Soc.* **201,** 202–206 (1786).
2. M. Born and E. Wolf, *Principles of Optics,* Pergamon Press, New York (1959).
3. A. Maréchal and G. W. Stroke, Sur l'origine des effets de polarization et de diffraction dans les réseaux optiques, *C. R. Acad. Sci. Paris B* **249,** 2042–2044 (1959).
4. P. Beckmann and A. Spizzicerio, *The Scattering of Electromagnetic Waves from Rough Surfaces,* Pergamon Press, New York (1963).
5. R. Madden and J. Strong: *Concepts of Classical Optics,* Freeman, San Francisco (1958).
6. O. M. Lord Rayleigh, On the dynamical theory of gratings, *Proc. Royal Soc.* (*London*) Ser. A **79,** 399–416 (1907).
7. M. Cadilhac, Some mathematical aspects of the grating theory, Chap. 2, in *Electromagnetic Theory of Gratings*, R. Petit, Ed. Springer-Verlag, Berlin (1980).
8. H. Ikuno and K. Yasuura, Improved point-matching method with application to scattering from a periodic surface, *IEEE Trans. Ant. Propag.* **AP-21,** 657–662 (1973).
9. (a) M. Nevière, G. Cerutti-Maori, and M. Cadilhac, Sur une nouvelle méthode de résolution du problème de la diffraction d'une onde plane par un réseau infiniment conducteur, *Opt. Commun.* **3,** 48–52 (1971); (b) M. Nevière, P. Vincent, and R. Petit, Sur la théorie du réseau conducteur et ses applications a l'optique, *Nouv. Rev. Opt.* **5,** 65–77 (1974); (c) P. Vincent, Differential methods, Chap. 4, in *Electromagnetic Theory of Gratings*, R. Petit, Ed. Springer-Verlag, Berlin, (1980).
10. L. Li, Formulation and comparison of two recursive matrix algorithms for modeling layered diffraction gratings, *J. Opt. Soc. Am. A* **13,** 1024–1035 (1956).
11. M. Nevière and F. Montiel, Electromagnetic theory of multilayer gratings and zone plates, Chap. 6, in *Multilayer and Grazing Incidence X-Ray/EUV Optics III*, R. B. Hoover and A. B. C. Walker, Eds. *Proc. SPIE* (1996).
12. A. K. Cousins and S. Gottschalk, Applications of the impedance formalism to diffraction gratings with multiple coating layers, *Appl. Opt.* **29,** 4268–4271 (1990).
13. M. Nevière, M. Cadilhac, and R. Petit, Applications of conformal mappings to the diffraction of electromagnetic waves by a grating, *IEEE Trans. Ant. Propag.* **AP-21,** 37–46 (1973).
14. M. G. Moharam and T. K. Gaylord, (a) Rigorous coupled-wave analysis of planar-grating diffraction, *J. Opt. Soc. Am.* **71,** 811–818 (1977); (b) Rigorous coupled-wave analysis of dielectric surface-relief gratings, *J. Opt. Soc. Am.* **72,** 1385–1392 (1982).
15. C. Botten, M. S. Craig, R. C. McPhedran, J. L. Adams, and J. R. Andrewartha, (a) The dielectric lamellar diffraction grating, *Opt. Acta* **28,** 413–428 (1981); (b) The finitely conducting lamellar diffraction grating, *Opt. Acta* **28,** 1087–1102 (1981).
16. (a) J. R. Andrewartha, G. H. Derrick, and R. C. McPhedran, A general modal theory for reflection gratings, *Opt. Acta* **28,** (11), 1501–1516 (1981); (b) J. Y. Suratteau, M. Cadilhac, and R. Petit, Sur la détermination numérique des efficacités de certain réseaux diélectriques profonds, *J. Optics* (Paris) **14,** 273–282 (1983).
17. L. Li, Multilayer modal method for diffraction gratings of arbitrary profile, depth, and permittivity, *J. Opt. Soc. Am. A* **10,** 2581–2591 (1993).
18. D. Maystre, (a) Sur la diffraction d'une onde plane par un réseau métallique de conductivité finie, *Opt. Commun.* **6,** 50–54 (1972); (b) A new general integral theory for dielectric coated gratings, *J. Opt. Soc. Am.* **68,** 490–495 (1978).
19. J. Chandezon, D. Maystre, G. Raoult, (a) A new theoretical method for diffraction gratings and its numerical application, *J. Optics* (Paris) **11,** 235–241 (1980); (b) J. Chandezon, M. T. Dupuis, G. Cornet, and D. Maystre, Multicoated gratings: A differential formalism applicable in the entire optical region, *J. Opt. Soc. Am.* **72,** 839–846 (1982).
20. G. Derrick, R. McPhedran, D. Maystre, and M. Nevière, Crossed gratings: A theory and its applications, *Appl. Phys.* **18,** 39–52 (1972).