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On the Limits of Validity of the Two-Wave Approximation in the Dynamical Theory of Electromagnetic Scattering by Periodic Dielectric Media

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Abstract. — We investigate the accuracy and limits of validity of the two-wave approximation in the dynamical theory of electromagnetic scattering by periodic dielectric media. The errors ensuing from the approximation are estimated by applying the dynamical theory to a scattering problem for which an alternative exact electromagnetic solution is available and comparing results. The conditions for applying the approximate theory and its accuracy are discussed in terms of concepts peculiar to the classical dynamical theory of the scattering of X-rays in crystals, such as the Ewald sphere in the reciprocal space and the resonance error. After introducing the basic equations of the dynamical theory of electromagnetic scattering by three dimensional periodic dielectric media, the theory is applied to the scattering by one-dimensional periodic layered structures where a rigorous analytical solution is available. The analysis of the errors involved in the two-wave approximation indicates that, in the general case, the quality of the approximation cannot be quantified in terms of just the resonance error but it is also strongly affected by the dielectric contrast. Simple formulae are reported yielding a reliable error estimate in many practical cases. An extension of the results to the two and three dimensional case is also provided. Finally, it is suggested that a modification of the boundary conditions which are usually enforced in the dynamical theory when solving the propagation equation could improve its accuracy and extend the limits of validity of the two-wave approximation.

1. Introduction

The propagation of electromagnetic waves in periodic media exhibits many interesting and potentially useful characteristics. Examples include the X-ray diffraction by crystals, light diffraction by the periodic strain variations accompanying a sound wave, total reflection of light in periodic layered media, holography. Many of these phenomena are currently employed in a variety of optical devices such as diffraction gratings, holograms, free-electron lasers,

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distributed-feedback lasers, distributed-Bragg-reflector lasers, high-reflectance Bragg mirrors, acousto-optic filters, and so on. In addition, interdisciplinary analogies also lead to new exciting areas of research. An example is the recent discovery of three-dimensionally periodic dielectric structures exhibiting what is called a *photonic band gap* [1,2], by analogy with electronic band gaps in semiconductor crystals.

The Theory of Dynamical Scattering (DST), originally proposed by Darwin [3], Ewald [4, 5] and Laue [6] in order to give a rigorous description of the X-ray diffraction by perfect crystals and later extended by Zachariasen [7], James [8,9] and Kato [10], has proved to be a powerful tool in the study of the propagation of electromagnetic radiation in periodic structures [11–13]. It has been successfully used also to describe diffraction of electrons [14] and neutrons [15] by perfect crystals, light diffraction by cholesteric liquid crystals [16] and, more recently, it has been extended to free [17] and guided [18] propagation of electromagnetic waves in periodic dielectric media from microwaves up to optical frequencies. Interesting effects admitting technological applications, such as the Borrmann effect, the Fankuchen effect, the Pendellösung effect, total reflection and angular amplification are expected in these different frequency ranges [8,9,11,12,16–18].

A dynamical diffraction theory of deformed crystals was developed by Takagi [20,21], Taupin [22] and later by Boeuf *et al.* [23], with a view to providing a rigorous theoretical description of the electromagnetic scattering by elastically bent perfect crystals such as curved crystal monochromators both in Laue and Bragg geometry. In analogy, a DST approach has been recently used [24] in order to study the effects involved in the dynamical diffraction of electromagnetic waves by weakly curved periodic layered media, in the frequency range extending from millimeter waves up to the optical spectrum. In particular, an interesting effect that was highlighted consists in the possibility of continuously sweeping the direction of the diffracted beam over a relatively wide angular range by controlling the frequency. This effect seems to be promising for those technological applications where a frequency-direction conversion is required.

The DST considers the total wave field inside the periodic medium, where diffraction is taking place, as a single entity. The sequence of formal steps consists in: setting down Maxwell's equations, introducing a periodic dielectric constant in order to describe the medium, assuming wave solutions consistent with the periodicity (i.e. in the form of a superposition of Bloch waves), obtaining a set of homogeneous linear equations for the ratio of the field amplitudes and writing down a determinant whose value must vanish for nontrivial solutions to exist, consequently constraining the wavevectors. The main question posed by this approach is the number of waves which must be considered in the field expansion in order to obtain a good approximation of the wave solution. In X-ray, neutron and electron diffraction by perfect crystals, the so called two-wave approach gives very often an excellent approximation of the total field [7,8,11,12]. This occurs when the two plane waves are resonantly coupled by Bragg's law since in this condition the amplitudes of the two waves become dominant over all others making up the total field. In the case of X-rays, this results from the small dielectric contrast with respect to empty space $\psi(\mathbf{r}) = \epsilon(\mathbf{r}) - 1$, whose magnitude is typically $10^{-4} - 10^{-6}$, which in turn is a consequence of the small perturbation produced by the electron density distribution of the crystalline material. This is not, however, the general case in the scattering of electromagnetic waves by periodic dielectric media [17]. The entity of the perturbation produced by the periodic variation $\Delta\epsilon(\mathbf{r})$ of the dielectric constant ϵ_1 of the unperturbed matrix can vary over a wide range of values. Since the two-wave approximation progressively deteriorates with increasing perturbation, the question arises as to the limits of validity and the degree of its accuracy as a function of the ratio $\Delta\epsilon(\mathbf{r})/\epsilon_1$. This is an important problem since the DST formalism is quite general and when even the two-wave approximation holds, the

mathematical expressions of the excited fields take the same form as derived in reference [17], and the predictions of the two-wave theory are reliable. It must also be stressed that even though the n -wave approximation gives a more accurate description, the complexity of the analysis greatly increases with the number n of waves considered and it is very hard to obtain an analytical solution when $n > 3$; in this case a sophisticated numerical approach is required [13]. In addition, useful insights may be provided into the more general problem of accuracy of the n -wave approximation.

The conditions of applicability of the theory and its accuracy are discussed in terms of concepts peculiar to the dynamical theory, such as the *Ewald sphere* in reciprocal space and the *resonance error*, which allow a meaningful physical interpretation of the results.

In the following, we first introduce the basic concepts of the DST of electromagnetic waves by periodic dielectric media. Then, the theory is applied to the case of electromagnetic scattering by the so called periodic layered media, i.e. one-dimensional periodic (1D) structures made up of alternating layers of non-magnetic lossless dielectric materials with different dielectric constants, for which a rigorous analytical solution is known. A comparison of the results deriving from the two different approaches shows the limits of validity and the accuracy of the two-wave approach.

2. Fundamental Equations of the Dynamical Theory

Consider a three-dimensional (3D) periodic dielectric medium. We write the dielectric constant $\epsilon(\mathbf{r})$ as

$$\epsilon(\mathbf{r}) = \epsilon_1 + \Delta\epsilon(\mathbf{r}) \quad (1)$$

where ϵ_1 is the unperturbed part of $\epsilon(\mathbf{r})$ and $\Delta\epsilon(\mathbf{r})$ is the triply periodic function representing the perturbation. In the DST the propagation of the electromagnetic field is described in terms of the displacement vector \mathbf{D} which satisfies the following differential equation [17]

$$\nabla^2 \mathbf{D} + \nabla \times \nabla \times (\psi \mathbf{D}) = \epsilon_1 \mu_0 \frac{\partial^2 \mathbf{D}}{\partial t^2} \quad (2)$$

where

$$\psi(\mathbf{r}) = 1 - \frac{\epsilon_1}{\epsilon(\mathbf{r})} \quad (3)$$

The function $\psi(\mathbf{r})$ is triply periodic and can be expanded in the Fourier series with Fourier coefficients ψ_H

$$\psi_H = \frac{1}{V} \int_V \psi(\mathbf{r}) \exp(2\pi i \mathbf{B}_H \cdot \mathbf{r}) dV \quad (4)$$

where V is the volume of the unit cell, \mathbf{B}_H is the reciprocal lattice vector associated to the triad of Miller indices $H = (h, k, l)$. The periodic nature of the medium makes it possible to express the general solution of equation (2) as a linear combination of Bloch waves

$$\mathbf{D}(\mathbf{r}, t) = \sum_H \mathbf{D}_H \exp[2\pi i (ft - \mathbf{K}_H \cdot \mathbf{r})] \quad (5)$$

where

$$\mathbf{K}_H = \mathbf{K}_0 + \mathbf{B}_H \quad (6)$$

and f is the frequency of the electromagnetic radiation.

The amplitudes of the wavevectors K_H can be conveniently written in terms of the modulus K of the wavevector of a plane wave propagating in an unbounded homogeneous medium with dielectric constant ϵ_1 ($K = f(\epsilon_1 \mu_0)^{1/2}$)

$$K_H = K(1 + \delta_H) \quad (7)$$

where δ_H is the so called *resonance error*.

By inserting equation (5) and the Fourier expansion of equation (3) into equation (2), an infinite set of linear homogeneous equations is obtained [7]

$$(K_H^2 - K^2)\mathbf{D}_H = K_H^2 \sum_L \psi_{H-L} \mathbf{D}_{L[H]} \quad (8)$$

where $\mathbf{D}_{L[H]}$ is the projection of \mathbf{D}_L perpendicular to \mathbf{K}_H . A given wavefield thus contains in general an infinite number of waves.

We are interested in the solution of equation (8) in the case when the periodic variation of the dielectric constant can be considered as a small perturbation. In this case it is possible, under certain conditions, that only two of the plane waves in equation (8) have significant amplitudes (two-wave approximation). A given wavefield thus contains a wave propagating along \mathbf{K}_0 (the incident wave) and a wave propagating along \mathbf{K}_H (the diffracted wave), that is, Bragg diffraction occurs. The moduli of the wavevectors \mathbf{K}_0 and \mathbf{K}_H are very close to K , resonance errors are small enough so that $(K_H^2 - K^2)/K_H^2 \approx 2\delta_H$ and we can write

$$\mathbf{D}_H = \frac{1}{2\delta_H} \sum_L \psi_{H-L} \mathbf{D}_{L[H]} \quad (9)$$

The last equation shows that a resonance effect is associated to the smallness of the resonance error, which makes the amplitudes of the corresponding waves dominant over all the others. The system (9) for the amplitudes D_0 and D_H of the wavefields then reduces to [7]

$$\begin{aligned} (\psi_0 - 2\delta_0)D_0 + P\psi_H D_H &= 0 \\ P\psi_H D_0 + (\psi_0 - 2\delta_H)D_H &= 0 \end{aligned} \quad (10)$$

where $\bar{H} = -H$, $P = 1$ ($P = \cos 2\theta$) for a polarization normal (parallel) to the plane \mathbf{K}_0 , \mathbf{K}_H and 2θ is the angle between \mathbf{K}_0 and \mathbf{K}_H . Equations (10) have a non trivial solution only if the determinant vanishes, which gives the dispersion equation

$$(\psi_0 - 2\delta_0)(\psi_0 - 2\delta_H) = P^2 |\psi_H|^2 \quad (11)$$

A linear relation between δ_H and δ_0 can be found by combining equations (6) and (7) and considering that the resonance errors δ_0 and δ_H are much smaller than unity. If \mathbf{K} indicates the wavevector of an incident plane wave entering the periodic structure through a plane boundary with unit inward normal \mathbf{n} and γ_0 is the direction cosine of the incident wave ($\gamma_0 = \mathbf{K} \cdot \mathbf{n}/K$), as long as the incidence angle is small enough so that the approximation $(1 + 2\delta_0/\gamma_0^2)^{1/2} \approx 1 + \delta_0/\gamma_0^2$ holds, the following linear relation between δ_H and δ_0 holds [7, 17]

$$\delta_H = \frac{1}{\beta} \delta_0 + \frac{\alpha}{2} \quad (12)$$

where

$$\begin{aligned} \frac{1}{\beta} &= 1 + \frac{B_H}{\mathbf{K} \cdot \mathbf{n}} \\ \alpha &= \frac{1}{K^2} (B_H^2 + 2\mathbf{K} \cdot \mathbf{B}_H) \end{aligned} \quad (13)$$

In particular, when the wavelength of the incident wave is varied while maintaining a fixed direction of incidence, equation (13) for α reduces to

$$\alpha = 4 \frac{\lambda - \lambda_B}{\lambda_B} \sin^2 \theta_B \tag{14}$$

where θ_B is the Bragg glancing angle, λ_B is the value of wavelength which satisfies the Bragg law with $\theta = \theta_B$ ($\lambda_B = 2d \sin \theta_B$) and λ is a neighbouring wavelength. By inserting equation (12) into equation (11), we obtain an equation in δ_0 , whose solutions can be written as [7]

$$\left. \begin{matrix} \delta_0' \\ \delta_0'' \end{matrix} \right\} = \frac{1}{2} \left[\psi_0 - \zeta \pm (q^2 + \zeta^2)^{1/2} \right] \tag{15}$$

where

$$\zeta = \frac{1 - \beta}{2} \psi_0 + \frac{\beta}{2} \alpha \qquad q = \beta |\psi_H|^2 \tag{16}$$

Introducing the variable $x = D_H/D_0$ and solving the system (10), two solutions x_1 and x_2 are obtained. Since there are two possible values for δ_0 , δ_H and for the amplitude ratio x , two internal incident waves and two internal diffracted waves are generated by the incident external wave with wavevector \mathbf{K} . The general expressions of the total incident and diffracted field are given, respectively, by

$$\begin{aligned} & e^{2\pi i(ft - \mathbf{K} \cdot \mathbf{r})} \left[D_0' e^{-i\phi_1 z} + D_0'' e^{-i\phi_2 z} \right] \\ & e^{2\pi i[ft - (\mathbf{K} + \mathbf{B}_H) \cdot \mathbf{r}]} \left[x_1 D_0' e^{-i\phi_1 z} + x_2 D_0'' e^{-i\phi_2 z} \right] \end{aligned} \tag{17}$$

where

$$\phi_1 = 2\pi K \delta_0' / \sin \theta \qquad \phi_2 = 2\pi K \delta_0'' / \sin \theta \tag{18}$$

It is possible to give a simple physical interpretation of the resonance error by using the construction involving the Ewald sphere in the reciprocal space [7,11,12] (see Fig. 1). According to equation (7) the modulus of the resonance error δ_H (or δ_0) represents the distance of the reciprocal lattice point H (or O) from the surface of the Ewald sphere, normalized to the radius K of the sphere. Only when the resonance error is very small, i.e. the points H and O are very close to the surface, the resonance coupling between incident and diffracted waves makes the amplitudes of the two waves dominant over all the others, thus justifying the two-wave approximation. In the next paragraphs we will try to answer the following question: how close to the surface the reciprocal lattice point H must be in order to obtain a two-wave approximation of the wave solution within a specified degree of precision?

3. Application of the DST to Periodic Layered Media

In order to answer the above question it is necessary to consider an electromagnetic problem which allows an exact solution and next compare the results with those expected by the DST. To this purpose we consider the wave propagation in a periodic layered medium made up of alternating layers of nonmagnetic lossless dielectric materials with different dielectric constants ϵ_1 and ϵ_2 (see Fig. 2a). In the unit cell it is (Fig. 2b)

$$\epsilon(z) = \begin{cases} \epsilon_2 & |z| < b/2 \\ \epsilon_1 & b/2 \leq |z| < \Lambda/2 \end{cases} \tag{19}$$

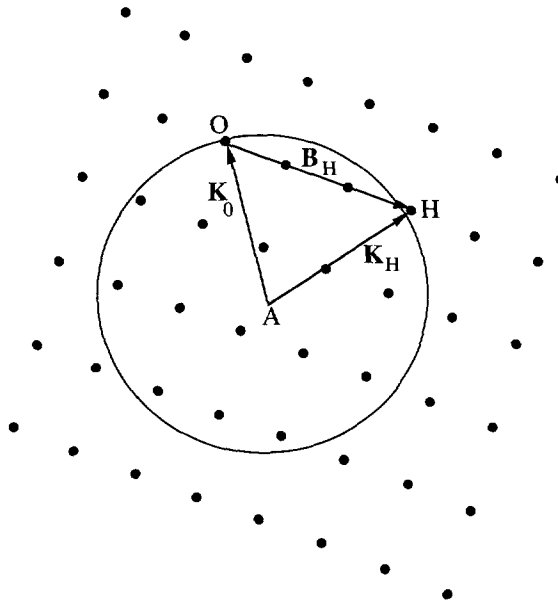


Fig. 1. — Ewald sphere in the reciprocal space. O and H are the origin and a point of the reciprocal lattice, respectively; A is the centre of the sphere and $AO = |\mathbf{K}_0|$ is the radius. \mathbf{K}_0 is the wavevector of the incident wave, $|\mathbf{K}_H|$ the wavevector of the diffracted wave and $|\mathbf{B}_H|$ is a vector of the reciprocal lattice. The modulus of the resonance error δ_H (or δ_O) represents the distance of the reciprocal lattice point H (or O) from the surface of the Ewald sphere, normalized to the radius of the sphere.

where the z -axis is normal to the layer interfaces and Λ is the period. In order to eliminate all the approximations which are not strictly connected to the two-wave choice of the solution, such as those related to the boundary conditions for the wavevectors on the limiting surfaces, we restrict the analysis to the case of normal incidence of a TE wave (i.e., normal polarization, $P = 1$). As a matter of convenience, we consider the material with dielectric constant ϵ_1 to be the matrix and the material with dielectric constant ϵ_2 the perturbation.

The most obvious and simple quantity to determine for comparing the two approaches is the reflectivity curve, i.e. the ratio of the reflected to the incident power as a function of the frequency.

The exact solution of the problem can be obtained following the approach described in references [25] and [26], which makes use of the translational matrix formalism. If we consider a portion L of the periodic structure consisting of N unit cells and faced at both ends, $z = 0$ and $z = L = N\Lambda$, to the homogeneous matrix, the following expression of the reflectivity R^2 is obtained

$$R^2 = \frac{|C|^2}{|C|^2 + \left[\frac{\sin(2\pi K' \Lambda)}{\sin(2N\pi K' \Lambda)} \right]^2} = \frac{|C|^2 \left[\frac{\sin(2N\pi K' \Lambda)}{\sin(2\pi K' \Lambda)} \right]^2}{|C|^2 \left[\frac{\sin(2N\pi K' \Lambda)}{\sin(2\pi K' \Lambda)} \right]^2 + 1} \quad (20)$$

where K' is the solution of the associated eigenvalue equation (Eq. (6.2 – 26) of Ref. [26]):

$$F(\bar{b}, \rho, \lambda_n) = \cos 2\pi K' \Lambda \quad (21)$$

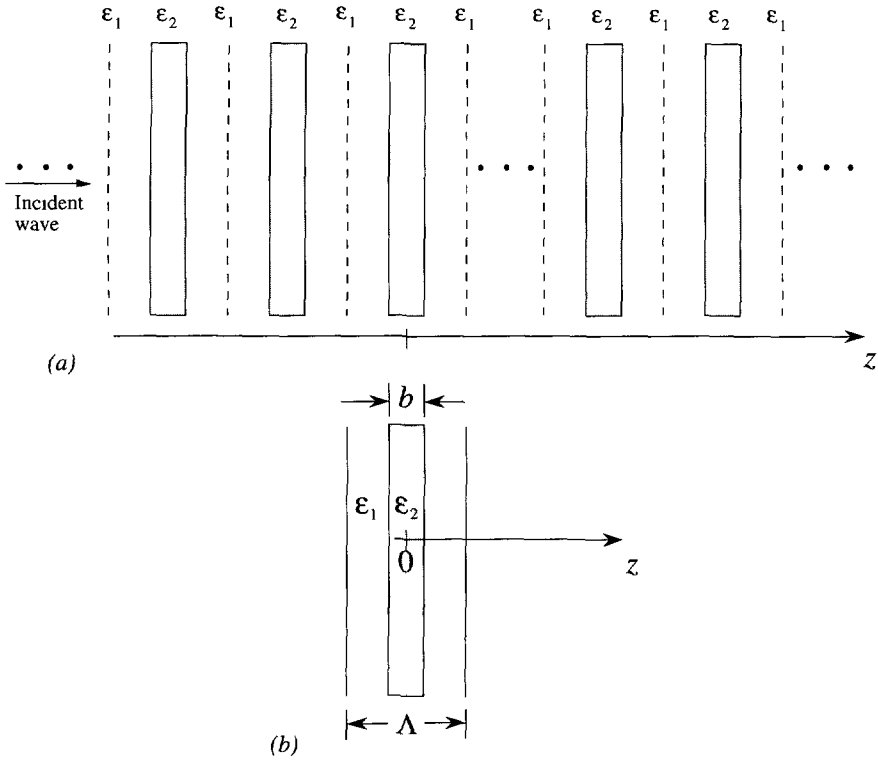


Fig. 2. — Schematic drawing of a periodic layered medium. a) The periodic structure consists of alternating layers of nonmagnetic lossless dielectric materials with different dielectric constants ϵ_1 and ϵ_2 . b) The unit cell of the 1D periodic structure.

where

$$F(\bar{b}, \rho, \lambda_n) = \cos\left(\frac{2\pi}{\lambda_n} \rho \bar{b}\right) \cos\left(\frac{2\pi}{\lambda_n} (1 - \bar{b})\right) - \frac{1}{2} \left(\rho + \frac{1}{\rho}\right) \sin\left(\frac{2\pi}{\lambda_n} \rho \bar{b}\right) \sin\left(\frac{2\pi}{\lambda_n} (1 - \bar{b})\right). \quad (22)$$

The term $|C|^2$ is related to the reflectivity $|R_u|^2$ of the single unit cell by the equation (Eq. (6.2 - 12) of Ref. [26])

$$|C|^2 = \frac{|R_u|^2}{1 - |R_u|^2} = \frac{1}{4} \left[\frac{n_2}{n_1} - \frac{n_1}{n_2} \right]^2 \sin^2 2\pi K_2 b = \frac{1}{4} \left[\rho - \frac{1}{\rho} \right]^2 \sin^2 \left(\frac{2\pi}{\lambda_n} \rho \bar{b} \right) \quad (23)$$

and $n_1 = \epsilon_1^{1/2}$, $n_2 = \epsilon_2^{1/2}$, $\rho = n_2/n_1 = (\epsilon_2/\epsilon_1)^{1/2}$, $\lambda_n = \lambda/\Lambda$, $\bar{b} = b/\Lambda$, $K_2 = f(\epsilon_2 \mu_0)^{1/2}$

The DST approach, on the other hand, follows the lines reported in the previous paragraph. In this case the vector \mathbf{B}_H of the one-dimensional reciprocal lattice is given by $\mathbf{B}_H = \mathbf{B}_h = (h/\Lambda)\mathbf{n}$, with $h = 0, \pm 1, \pm 2, \dots$, and the function $\psi(\mathbf{r})$ is periodic only with respect to z . By performing the integration (4) while fixing the origin of the coordinate system in the centre of the unit cell (Fig. 2b), the Fourier coefficients ψ_h take the form

$$\psi_h = \frac{b}{\Lambda} \left(1 - \frac{\epsilon_1}{\epsilon_2} \right) \frac{\sin(h\pi b/\Lambda)}{(h\pi b/\Lambda)} = \bar{b} \left(1 - \frac{1}{\rho^2} \right) \frac{\sin(h\pi \bar{b})}{(h\pi \bar{b})} \quad (24)$$

The two-wave approximation can be used when the reciprocal lattice point H is close to surface of the Ewald sphere, i.e. when $K_H \approx K_0 \approx K$. The latter condition is verified when the wavelength λ of the incident radiation is close to the value λ_B which satisfies the Bragg's law, i.e. $h\lambda_B = 2\Lambda$. In the DST, the reflectivity is generally expressed as a function of a dimensionless parameter y which depends on the wavelength and measures the deviation from the Bragg condition for the diffraction [7, 17, 18]. For normal incidence, normal polarization, and taking $h = 1$, the expression of y is given by

$$y = \frac{\zeta}{|\beta|^{1/2} P |\psi_h|} = \frac{\psi_0 - 2(\lambda - \lambda_B)/\lambda_B}{|\psi_1|} \quad (25)$$

By using equations (25) and (16) it is possible to express the resonance errors in equation (15) in terms of y , ψ_0 and $|\psi_h|$ as follows

$$\left. \begin{array}{l} \delta_0' \\ \delta_0'' \end{array} \right\} = \frac{1}{2} \psi_0 + \frac{1}{2} |\psi_h| \left[-y \pm (y^2 - 1)^{1/2} \right] \quad (26)$$

This equation allows us to calculate the resonance error as a function of the wavelength deviation from the Bragg wavelength. Considering equation (26) and the expression of ψ_h , it is immediate to observe that in the y -range commonly considered in the DST, i.e. Δy corresponding to a few units around $y = 0$, the order of magnitude of the resonance errors is the same as ψ_0 . For this reason and considering also that ψ_0 does not depend on the frequency and it is related to the geometrical and physical parameters of the structure more simply than δ_0 , the two-wave approximation will be considered in the following in terms of the magnitude of ψ_0 rather than δ_0 .

The ratio of the diffracted wave amplitude D_H to the external incident wave amplitude D_e^0 at the input surface is obtained from equations (17), after imposing the following boundary conditions over the two limiting surfaces [7, 17]

$$\begin{aligned} D_0' + D_0'' &= E_e^0 \\ x_1 D_0' e^{-i\varphi_1 L} + x_2 D_0'' e^{-i\varphi_2 L} &= 0 \end{aligned} \quad (27)$$

where E_e^0 is the electric field of the external incident wave. The reflectivity R'^2 is calculated as the ratio $|D_H/E_e^0|^2$

$$R'^2 = \frac{\sin^2 [A(y^2 - 1)^{1/2}]}{(y^2 - 1) + \sin^2 [A(y^2 - 1)^{1/2}]} \quad (28)$$

where

$$A = \pi |\beta|^{1/2} P K |\psi_h| L / \sin \theta \quad (29)$$

which is valid both for $|y| > 1$ and $|y| < 1$, being in the latter case $\sin^2 [A(y^2 - 1)^{1/2}] = \sinh^2 [A(1 - y^2)^{1/2}]$.

Equality between equations (20) and (28) requires the following two conditions to be satisfied

$$A \sqrt{y^2 - 1} = 2N\pi K' \Lambda \quad (30)$$

$$\frac{|C|}{|\sin 2\pi K' \Lambda|} = \frac{1}{\sqrt{y^2 - 1}} \quad (31)$$

Consider equalities (30) and (31) separately. The term $A \sqrt{y^2 - 1}$ can be explicitly written in terms of the quantities appearing in equations (20-23) in the form

$$A \sqrt{y^2 - 1} = N \Lambda \frac{\pi}{\lambda} S(\bar{b}, \rho, \lambda_n) \quad (32)$$

where

$$S(\bar{b}, \rho, \lambda_n) = \sqrt{[\bar{b}(1 - 1/\rho^2) - (\lambda_n - 2)]^2 - \left[\bar{b}(1 - 1/\rho^2) \frac{\sin \pi \bar{b}}{\pi \bar{b}}\right]^2} \quad (33)$$

If we indicate by

$$Q(\bar{b}, \rho, \lambda_n) = \cos \left[\frac{\pi}{\lambda_n} S(\bar{b}, \rho, \lambda_n) \right] \quad (34)$$

equation (31) requires the following condition to be verified

$$|Q(\bar{b}, \rho, \lambda_n)| = |F(\bar{b}, \rho, \lambda_n)| \quad (35)$$

The strength of the perturbation is measured by the two parameters ρ and \bar{b} . Small perturbation means that either one of the two conditions, $\rho \approx 1$ and $\bar{b} \approx 0$, is verified. For a given wavelength, i.e. once fixed the normalized wavelength λ_n , Q and F are both functions of the two variables ρ and \bar{b} . As shown in the following, the first two terms of the Taylor expansion of the two members in equation (35) are the same in a neighbourhood of the point ($\rho = 1, \bar{b}$), with \bar{b} assuming any value between 0 and 1. In fact, to the first order approximation, it is

$$F(\bar{b}, \rho, \lambda_n) = \cos \frac{2\pi}{\lambda_n} - \frac{2\pi}{\lambda_n} (\rho - 1) \bar{b} \sin \frac{2\pi}{\lambda_n} \quad (36a)$$

$$Q(\bar{b}, \rho, \lambda_n) = -\cos \frac{2\pi}{\lambda_n} + \frac{2\pi}{\lambda_n} (\rho - 1) \bar{b} \sin \frac{2\pi}{\lambda_n} \quad (36b)$$

Differently, the first order Taylor expansion in a neighbourhood of ($\rho, \bar{b} = 0$) for any given value of ρ gives

$$F(\bar{b}, \rho, \lambda_n) = \cos \frac{2\pi}{\lambda_n} + \frac{\pi}{\lambda_n} (1 - \rho^2) \bar{b} \sin \frac{2\pi}{\lambda_n} \quad (37a)$$

$$Q(\bar{b}, \rho, \lambda_n) = -\cos \frac{2\pi}{\lambda_n} + \frac{\pi}{\lambda_n} (1 - \rho^{-2}) \bar{b} \sin \frac{2\pi}{\lambda_n} \quad (37b)$$

from which it follows that the moduli of F and Q become equal only as ρ approaches 1. In addition, equations (37a,b) show that while the dependence of the two functions F and Q on the parameter \bar{b} is the same to the first order, the dependence on ρ is different. This result indicates that the dependence on the dielectric step ρ is the dominant factor in determining the limits of validity of the two-wave approximation. Although this conclusion is physically reasonable, however it is not obvious *a priori* because in all the equations of the DST the effects of the perturbation are expressed in terms of the parameters ψ_0 and ψ_H which combine the effects of \bar{b} and ρ ; accordingly, the separate effects of \bar{b} and ρ are not distinguishable.

We define the relative error e_1 involved in the calculation of the eigenvalues of the unit cell as

$$e_1 = \left| 1 - \left| \frac{Q(\bar{b}, \rho, \lambda_n)}{F(\bar{b}, \rho, \lambda_n)} \right| \right| \quad (38)$$

Formulae (37a,b) allow us to give an estimate of e_1 by considering the first order approximation of the ratio Q/F with respect to the variable \bar{b} .

$$e_1 \approx \left| \frac{\pi}{\lambda_n} [2 - (\rho^2 + \rho^{-2})] \bar{b} \tan \frac{2\pi}{\lambda_n} \right| = \left| \frac{\pi}{\lambda_n} (1 - \rho^2) \psi_0 \tan \frac{2\pi}{\lambda_n} \right| \quad (39)$$

The above equation is derived under the hypothesis that the argument of the modulus in equation (39) is lower than 1, as it is in a wavelength range centred about $\lambda_n = 2$ when ($\rho - 1$)

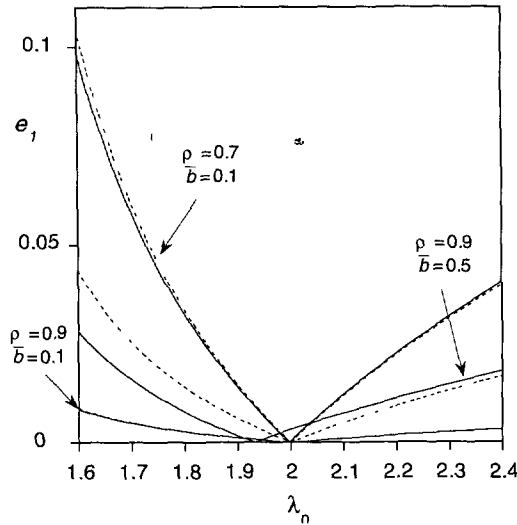


Fig. 3. — Comparison between the error e_1 calculated by its exact expression equation (38) (solid line) and by the approximated formula equation (39) (dashed line) for different values of ρ and \bar{b} .

and \bar{b} are small enough. The formula shows that the error is very small when $\lambda_n \approx 2$ (i.e. when the Bragg's law is close to be satisfied) and becomes zero when $\lambda_n = 2$ (the Bragg's law is exactly satisfied). In spite of its simplicity, formula (39) provides a good estimate of e_1 ; in fact, as shown in Figure 3, where it is compared with the exact expression of e_1 (Eq. 38) for different values of ρ and \bar{b} , equation (39) gives satisfactory results even in the worst case, i.e. $\bar{b} = 0.5$ (for larger values of \bar{b} the role of the two materials ϵ_1 and ϵ_2 could be more conveniently exchanged). Accordingly, equation (39) can be used to estimate the error occurring in periodic structures having more complicated dielectric profiles (such as those realized in the fabrication of actual periodic structures for optical applications) for which it is possible to calculate ψ_0 and to give at least an estimate of ρ . Finally, we note that all the equations in the present analysis are valid both for $0 \leq \rho \leq 1$ and for $\rho \geq 1$. However, for the sake of brevity, only results concerning the first case will be shown in the following.

So far we have considered the approximation involved in determining the eigenvalues of the periodic structure. Now, the accuracy of equation (31) is checked. Although the exact determination of the eigenvalue $2\pi K' \Lambda$ requires the solution of equation (21), we have just seen that this eigenvalue is accurately approximated by (30), i.e. (see also Eq. (32))

$$\sin 2\pi K' \Lambda \approx \sin \left[\frac{\pi}{\lambda_n} S(\bar{b}, \rho, \lambda_n) \right] \quad (40)$$

When \bar{b} is small, by considering the first order Taylor expansion of each member of equation (31), we get

$$\frac{|C|}{|\sin 2\pi K' \Lambda|} \approx \left| \frac{\frac{\pi}{\lambda_n} (\rho^2 - 1) \bar{b}}{\sin \left[\frac{\pi}{\lambda_n} (\lambda_n - 2) \right]} \right| \quad (41a)$$

$$\frac{1}{|\sqrt{y^2 - 1}|} \approx \left| \frac{1 - \rho^{-2}}{\lambda_n - 2} \right| \quad (41b)$$

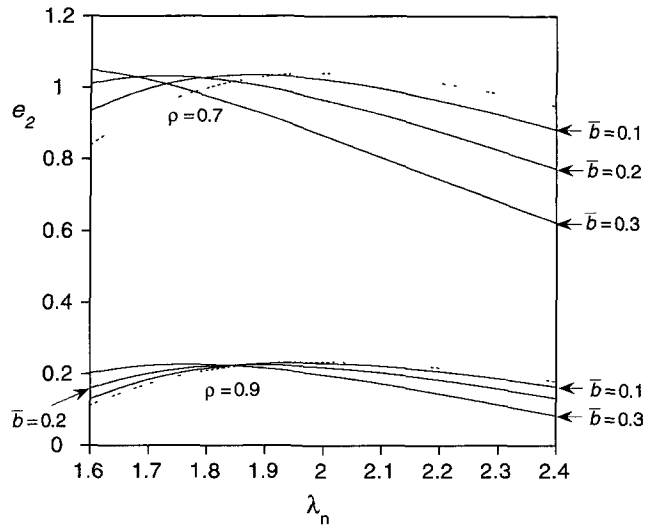


Fig. 4. — Comparison between the error e_2 calculated by its exact expression equation (42) (solid line) and by the approximated formula equation (43) (dashed line) for different values of ρ and \bar{b} .

respectively. Accordingly, the relative error e_2 involved in the approximation of the amplitude of the reflectivity and expressed as

$$e_2 = \left| 1 - \frac{\sin 2\pi K' \Lambda}{|C| \sqrt{y^2 - 1}} \right| \tag{42}$$

can be written as

$$e_2 \approx \left| 1 - \frac{\sin \frac{\pi}{\lambda_n} (\lambda_n - 2) \frac{1 - \rho^{-2}}{\rho^2 - 1}}{\frac{\pi}{\lambda_n} (\lambda_n - 2)} \right| \tag{43}$$

The comparison for different values of \bar{b} between e_2 as obtained from equation (43) and its exact expression (42) is shown in Figure 4; the approximation is not as good as in the case of e_1 and it gives satisfactory results only when $\bar{b} \leq 0.2$. A comparison between Figure 3 and Figure 4 shows that e_2 is always greater than e_1 over the whole range of wavelengths considered. In addition, for relatively small values of the difference $|\rho - 1|$ (less than about 10^{-2} , e_2 is dominant over e_1 . For these reasons, in determining the accuracy of the wave approximation it is sufficient to consider the contribution of e_2 . Furthermore, the nature of the two errors, e_1 and e_2 , is quite different. While e_1 measures the error in the argument of the sinusoidal functions of the reflectivity curve or, equivalently, the error involved in the calculation of the eigenvalues of the cell, e_2 is connected to the error in the amplitude of the reflectivity curve; e_1 is then strictly associated to the two-wave truncation in the total wavefield expansion whereas e_2 is mainly affected by the further approximation introduced through the boundary conditions (27), i.e. neglecting the reflected wave at the input surface and assuming the dielectric constant step through the limiting surface enough small to justify the use of the **D** vector in the continuity equation for the tangential electric field. Accordingly, the error e_2 must be considered to estimate the overall degree of approximation whereas e_1 seems to be

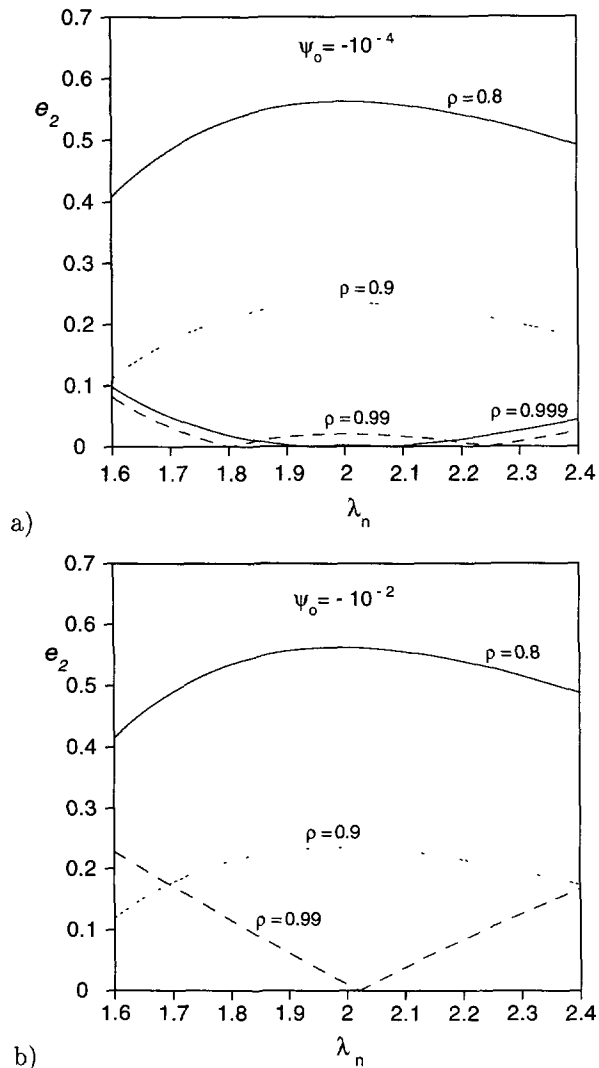


Fig. 5. — The behaviour of e_2 as a function of λ_n for different values of ρ and ψ_0 : a) $\psi_0 = -10^{-4}$; b) $\psi_0 = -10^{-2}$

more adequate to determine the accuracy of approximation which is strictly connected to the two-wave expansion of the wavefield.

The behaviour of e_2 and e_1 as a function of λ_n for different values of ρ and ψ_0 is reported in Figures 5 and 6, respectively. We observe that, once fixed ψ_0 , each given value of ρ determines a corresponding value of \bar{b} ; in addition, when ψ_0 is negative (i.e. $\rho < 1$), reducing ρ corresponds to reducing \bar{b} . Curves corresponding to positive values of ψ_0 (i.e. $\rho > 1$) are not reported in the figures since, for the same values of $|\psi_0|$ and $|\rho - 1|$, we found the same order of magnitude of the errors and only slight differences in the behaviour of the curves.

The consideration of Figures 5, 6 highlights the following results. The maximum error e_2 involved in the two-wave approximation cannot be expressed only in terms of the magnitude

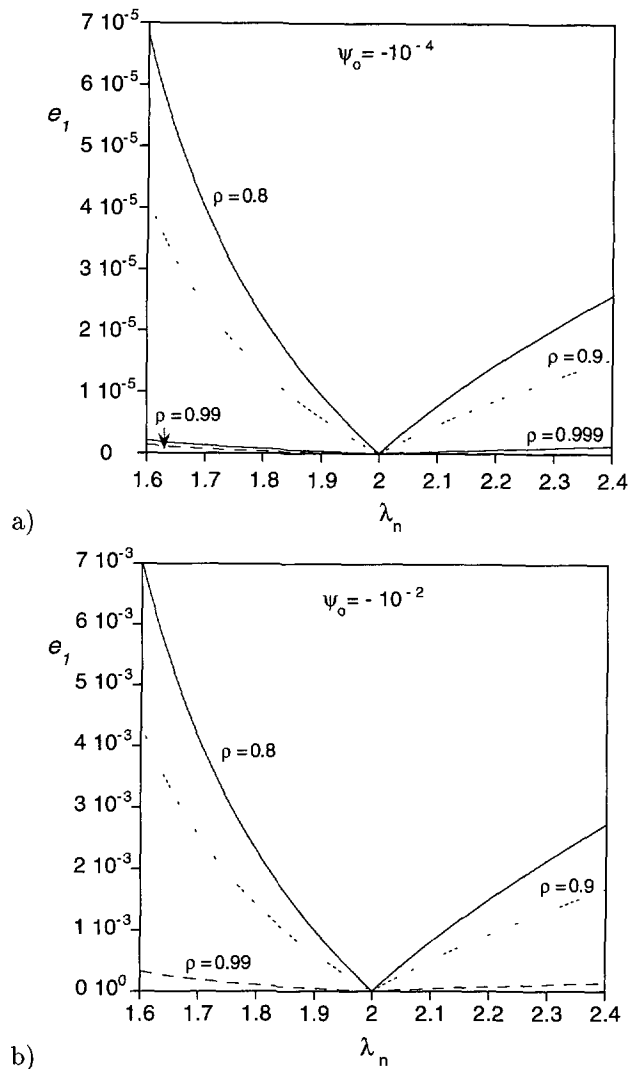


Fig. 6. — The behaviour of e_1 as a function of λ_n for different values of ρ and ψ_0 : a) $\psi_0 = -10^{-4}$; b) $\psi_0 = -10^{-2}$

of ψ_0 (hence of the resonance error) but also requires the specification of an upper limit for the quantity $1 - \rho$. In other terms, it is not sufficient to assign the magnitude of the resonance error to provide an estimate of the accuracy of the approximation; depending on the value of ρ , the same resonance error leads to approximation errors varying from a few percent to more than 50 percent. Using the curves reported in Figure 5 it is a possible quantitative evaluation of the maximum error e_2 . As an example, Figure 5a shows that when $\psi_0 = -10^{-4}$ and the difference $1 - \rho$ does not exceed 10^{-2} , e_2 is lower than 2% in the range of λ_n between 1.8 and 2.2 which corresponds to a fractional normalized bandwidth $\Delta\lambda_n/\lambda_n = 0.2$. Value of ψ_0 of this order of magnitude and even lower ($10^{-4} - 10^{-6}$) are usually found in X-ray, neutron and electron diffraction by perfect crystals where the two-wave approximation is well known to give

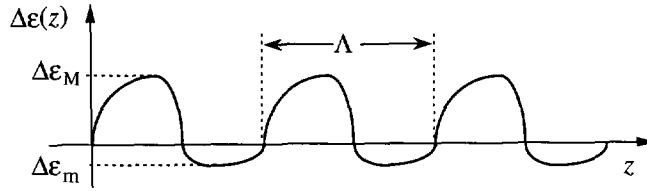


Fig. 7. — 1D periodic layered structure with a general z -dependence of the dielectric constant profile within the unit cell. $\Delta\epsilon_M$ and $\Delta\epsilon_m$ are the maximum and the minimum value of $\Delta\epsilon$ in the unit cell, respectively.

a very accurate description of the diffraction phenomena. The present results show that the same holds for the scattering of electromagnetic waves by periodic dielectric media provided that the perturbation is small enough to make $|\psi_0|$ lower than $\approx 10^{-4}$ and the difference $|1 - \rho|$ lower than $\approx 10^{-2}$. Figure 5b shows that good results are possible even for values of ψ_0 much higher than those typically encountered in X-ray, neutron and electron dynamical diffraction, provided that $|\rho - 1|$ is sufficiently small. In particular, we see that if $|\rho - 1| < 10^{-2}$ the error is lower than 5% percent in a relatively wide wavelength range ($\Delta\lambda_n/\lambda_n \approx 0.1$) and better performances are achieved with smaller values of $|\rho - 1|$.

Similar considerations hold for the error e_1 . In this case, however, the maximum error is at least two orders of magnitude lower than the corresponding e_2 .

The above results concerning the limits of validity of the two-wave approximation in 1D periodic layered structures can be extended to the general case of 1D periodic media with any z -dependence of the dielectric constant profile within the unit cell. To this purpose it is necessary to identify the parameters which play the role of \bar{b} and ρ in this approach. In the general case, the dielectric constant $\epsilon(z)$ of the 1D periodic structure within the unit cell can be written as

$$\epsilon(z) = \epsilon_1 + \Delta\epsilon(z) \quad (44)$$

where the perturbed part $\Delta\epsilon(z)$ is any function of z (see Fig. 7) and is small with respect to ϵ_1 . The Fourier coefficient ψ_0 is a complex number and the accuracy of the approximation must be discussed in terms of its modulus, $|\psi_0|$. Since the error depends on ρ more strongly than on \bar{b} , we can replace the original structure by a periodic layered one characterized by the parameters ρ and \bar{b} , given by the following equations

$$\rho = \left(\frac{\Delta\epsilon_M - \Delta\epsilon_m}{\epsilon_1} \right)^{1/2} \quad (45)$$

$$\bar{b} = \frac{|\psi_0|}{1 - \rho^{-2}} \quad (46)$$

where $\Delta\epsilon_M$ and $\Delta\epsilon_m$ are the maximum and the minimum value of $\Delta\epsilon$ in the unit cell, respectively. The new structure is actually more perturbed than the original one and, accordingly, an estimate of the maximum error based upon this structure will provide an upper limit for the real error in the original structure.

Finally, a simple extension of the results to 2D and 3D periodic dielectric structures is possible by considering an *equivalent* 1D structure where (according to the general definition of the Fourier coefficients $|\psi_H|$ in equation (4)) the quantity \bar{b} is given by the perturbed surface fraction of the total unit cell surface (2D case) or the perturbed volume fraction of the total unit cell volume (3D case). Again, this result will provide an over-estimate of the actual error

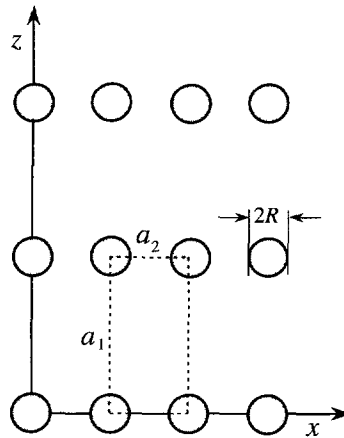


Fig. 8. — The 2D grating of cylindrical holes ($\epsilon_2 = 1$) with circular cross section (radius $R = 0.75$ mm) of the experiment reported in reference [18]. The holes are made on a dielectric matrix of polyethylene ($\epsilon_1 = 2.345$). The lattice parameters of the unit cell are $a_1 = 15.1$ mm and $a_2 = 3.1$ mm.

in that if $|\psi_0|$ and ρ satisfy the limitations above stated, the maximum error will be the one calculated for the 1D case. However in this case, because of the different dimensionality of the structure, a given combination of $|\psi_0|$ and ρ could result in actual errors much lower than the maximum estimated. An example of this is given by the results of the experiment described in reference [18]. The structure considered in this experiment consists of a 2D grating of cylindrical holes ($\epsilon_2 = 1$) with circular cross section (radius $R = 0.75$ mm), made on a dielectric matrix of polyethylene ($\epsilon_1 = 2.345$). The lattice parameters of the unit cell (see Fig. 8) are $a_1 = 15.1$ mm and $a_2 = 3.1$ mm. The expression of $|\psi_0|$ for this structure is

$$\psi_0 = \frac{\pi R^2}{a_1 a_2} \left(1 - \frac{\epsilon_1}{\epsilon_2} \right) = \frac{\pi R^2}{a_1 a_2} (1 - \rho^{-2}) \quad (47)$$

The value of \bar{b} is given by the ratio of the cross section of the circular hole to the total surface of the unit cell, i.e. $\bar{b} = \pi R^2 / (a_1 a_2) = 3.775 \times 10^{-2}$, $\rho = (\epsilon_2 / \epsilon_1)^{1/2} = 0.653$ and $\psi_0 = -5.077 \times 10^{-2}$. The errors e_1 , e_2 obtained with these values of ψ_0 and ρ over the whole experimental frequency range investigated (7.4 GHz – 8.6 GHz) are reported in Figure 9. We observe that even if e_1 is less than 3% over the whole frequency range the amplitude error is very high. Such a high value of the error is not confirmed by the experimental evidence [18] which, on the contrary, indicates a good agreement over the whole frequency range between the experimental reflectivity curve and the theoretical one (calculated in the framework of the two-wave approximation) as shown in Figure 10. The probable reason is that the 1D equivalent structure considered is *too severe* in that it leads to an excessive over-estimate of the error. An alternative and more reliable estimate of ρ can be obtained by considering the 1D equivalent model of the real actual 2D structure reported in Figure 11, where $\langle \epsilon \rangle$ is the weighted average of the dielectric constant over the rectangular surface of dimensions $a_2 \times (2R)$. In this way we obtain $\rho = 0.884$, and \bar{b} is then calculated as $\bar{b} = \frac{\psi_0}{1 - \rho^{-2}} = 0.181$. With these values, the maximum estimated error greatly reduces as shown by Figure 12, and a reasonable agreement with the experimental results is found.

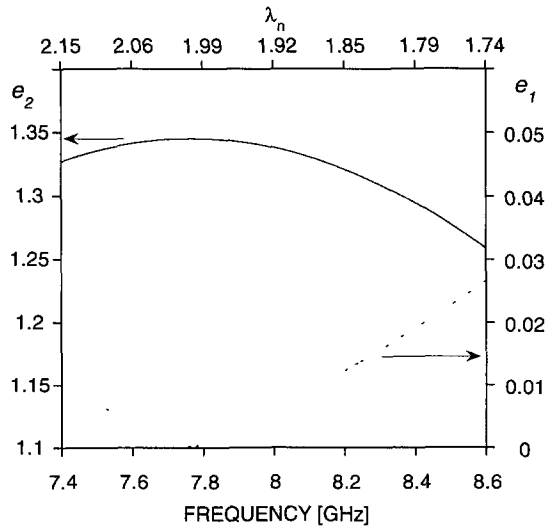


Fig. 9. — The behaviour of the errors e_1 (dotted line) and e_2 (solid line) over the whole experimental frequency range investigated. Here λ_n is the guide wavelength of the TE_{10} mode propagating in the rectangular waveguide used in the experiment (see Ref. [18]) normalized to $\Lambda = a_1$. Note that the scale λ_n is not linearly related to the frequency one (Eq. (2.72) in Ref. [18]).

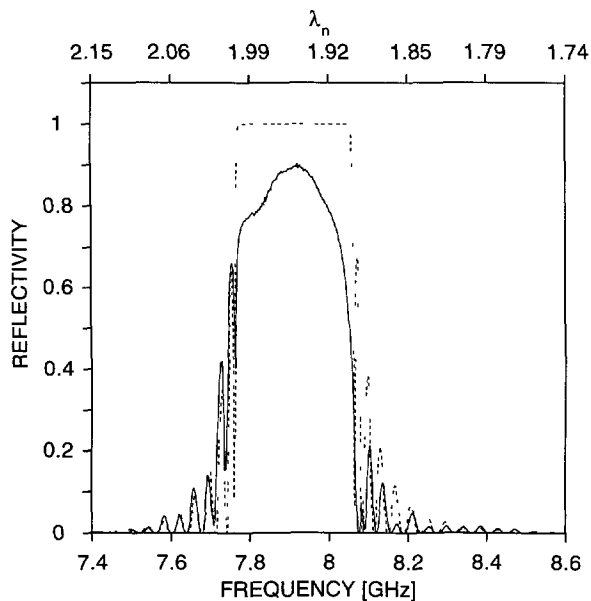


Fig. 10. — Comparison between the experimental reflectivity curve (solid line, from Ref. [18]) and the theoretical one obtained by the DST in the framework of the two-wave approximation (dotted line). For the λ_n scale, see the caption of Figure 9.

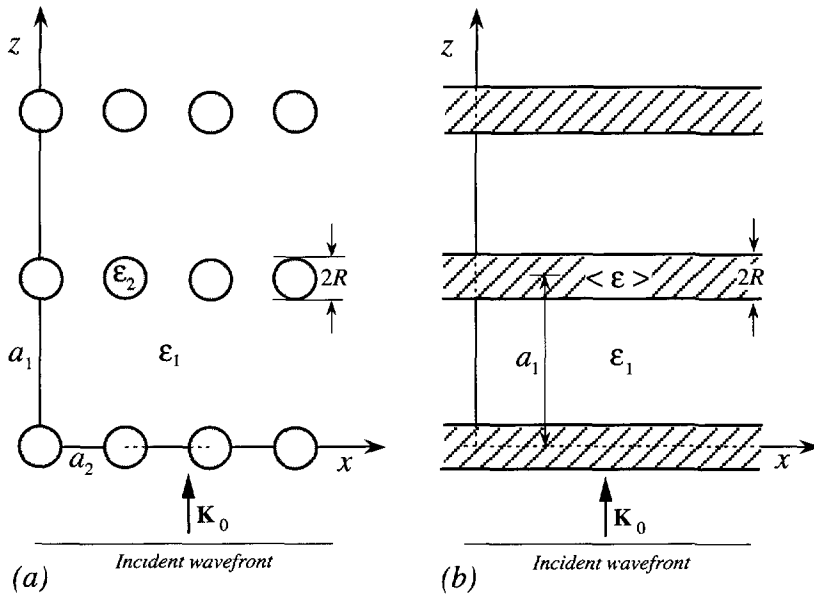


Fig. 11. — The 1D equivalent model (part(b)) of the 2D periodic structure of Figure 8 (part(a)); $\langle \epsilon \rangle$ is the weighted average of the dielectric constant over the rectangular surface of dimensions $a_2 \times (2R)$, i.e. $\langle \epsilon \rangle = [\epsilon_2 \pi R^2 + \epsilon_1 (2Ra_2 - \pi R^2)] / (2Ra_2)$.

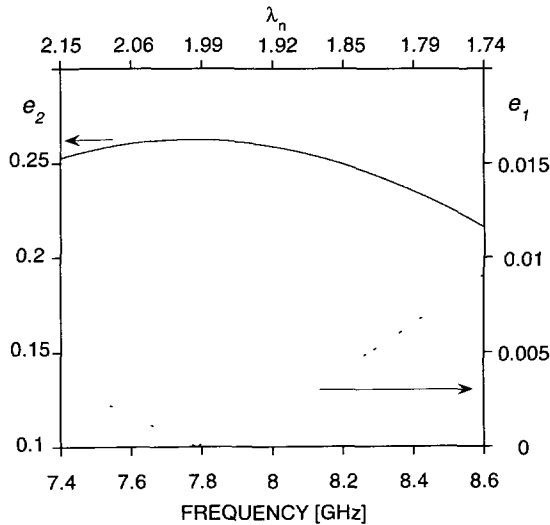


Fig. 12. — The behaviour of e_1 (dotted line) and e_2 (solid line) over the whole experimental frequency range investigated, obtained by considering the 1D equivalent model of the original 2D structure, i.e. $\rho = 0.884$ and $\bar{b} = 0.181$. For the λ_n scale. see the caption of Figure 9

Finally, a comparison between the experimental and the theoretical curve in Figure 10 indicates that the agreement is much better for the positions of the peaks than for their amplitudes. This experimental finding confirms the smallness of e_1 with respect to e_2 shown by the theoretical analysis in this paper.

4. Conclusions

The analysis of the errors connected to the two-wave approximation in the DST of electromagnetic waves by periodic dielectric media has shown that, in the general case, it is not possible to quantify the goodness of the approximation in terms of only the resonance errors. How close to the Ewald sphere the reciprocal lattice points must be to produce the strong resonance effect which justifies the approximation is a question which does not allow an absolute answer but is strictly related to the nature of the perturbation. In particular, it has been shown that the dielectric constant step, together with the resonance error, plays the main role in determining the limits of validity of the classical two-wave approach of the DST. Accordingly, a different behaviour is exhibited with respect to the case of X-ray, neutron and electron diffraction by perfect crystals where the entity of the perturbation is always very small. In the scattering of electromagnetic waves, resonance error of the order of 10^{-4} and even lower could not be sufficient to justify the approximation if the dielectric constant step is too high. On the other hand, resonance errors of the order of 10^{-2} and even larger can give rise to satisfactory results provided that the dielectric constant step $|\rho - 1|$ is small enough. The analysis developed and the formulae obtained for the errors e_1 and e_2 make it possible a quantitative estimate of the accuracy of the approximation for a given scattering problem. Finally, we showed that the accuracy of the two-wave DST is limited by the error e_2 which, differently from e_1 , is strongly affected by the further approximations introduced through the boundary conditions. Since e_1 is typically orders of magnitude lower than e_2 , the accuracy of the approximation which is strictly related to the two-wave truncation of the field, measured essentially by e_1 , is much better. This is also confirmed by the results of the experiment performed on a 2D periodic dielectric structure at microwave frequencies. Accordingly, better results could be obtained within the two-wave DST approach by a proper modification of the boundary conditions in the solution of the propagation equation.

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