SECOND ORDER APPROXIMATION FOR BAND GAP CHARACTERIZATION OF ONE-DIMENSIONAL DIELECTRIC OMNIDIRECTIONAL REFLECTOR

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A derivation of approximate analytical expressions for band edges $\omega^\pm$ of the first band gap of a multilayer periodic structure is presented for both TE and TM waves at arbitrary angles of incidence. It is found that the approximate expressions give an excellent agreement with the numerical results as verified by the band edge variation with respect to the filling fraction $\nu = \frac{d_2}{d}$ and refractive index contrast Δn . The analytical expressions for the band edges are further employed to derive a semi numerical optimization of the relative gap width $\xi = \frac{\Delta\omega}{\langle\omega\rangle}$ with respect to the filling fraction ν . The result is again shown to be in good agreement with the numerical result.

Keywords: One-dimensional grating; photonic band gap; omnidirectional reflector; band-edge optimization.

1. Introduction

It is well known that reflectors or mirrors are important elements in integrated optics devices. While being easier to fabricate, metallic mirrors generally suffer from undesirable absorption and heating effects.¹ This problem was principally overcome by the use of optical gratings made of dielectric materials which are practically lossless. Its near perfect reflection property is characterized by the existence of photonic band gap (PBG) covering a certain range of frequencies for a certain propagation direction. A **complete photonic band gap** (CPBG) emerges when the band gaps overlap for all directions of incidence and polarizations. A photonic component with this characteristic is known as omnidirectional reflector (ODR). Since the introduction of photonic crystal in 1987,^{2,3} it was suggested that only 3D PC was capable of ODR performance.⁴ Unfortunately, current technology is restricted to the fabrication of such devices operating in the microwave region only.^{5,6} Recent theoretical

and experimental investigations have nevertheless shown that even one-dimensional photonic crystals are capable of exhibiting a complete photonic band gaps.^{1,7} This is achieved by a structure made of a finite number of alternating dielectric slabs of alternating refractive indices n_1 and n_2 embedded in a background medium with refractive index n_0 satisfying $n_0 < n_1 < n_2$.

Being the boundaries of a photonic band gap, the band edges constitute an important set of design parameters of an ODR. Due to complexity of the dispersion relation defining the band edges, their exact closed form expressions are simply impossible to derive. Recently Lekner⁸ proposed an approximate analytical expression for these band edges. However, further examination of this work shows that the proposed expression does not yield a correct behavior and values of the band edges as compared with the exact numerical results for certain 1D multilayer structures. Aside from those discrepancies, the most troubling result was that the proposed expression gives a very different behavior of the upper band edge values for the TE polarized waves, implying a closing gap at large incidence angle, in contrary to the general physical understanding of reflection property of the grating system. This behavior apparently arises from the use of an inappropriate assumption in the approximation.

The present paper reports on the results of a further analysis of the approximate band edge expressions and the formulation of correct expressions for the band edges of the 1D omnidirectional reflector reported previously.⁹ An optimization scheme for maximizing the omnidirectional band gap with respect to the geometrical parameters of the system is also presented in this work.

2. Oblique Incidence Band Edge Approximation

As implied in the Introduction, a most important aspect in ODR design is the dependence of the band edges on the angle of incidence. In the present work only the first band gap is considered. The band edges are determined from the dispersion relation obtained by the standard transfer matrix approach¹⁰ as follows,

$$\cos q_1 \cos q_2 - \Xi_{12} \sin q_1 \sin q_2 = \cos(\mathbb{K}d), \quad (1)$$

where $\mathbb{K}$ is the Bloch wave number, the period $d = d_1 + d_2$ is the sum of thicknesses of the two layers, and

$$q_j = \frac{\omega}{c} D_j, \quad D_j = d_j n_j \cos \theta_j, \quad (2)$$

with θ_j denoting the incident angle from the j -th layer as depicted in Fig. 1, while

$$\Xi_{12} = \frac{1}{2} \left(\alpha_{12} + \frac{1}{\alpha_{12}} \right). \quad (3)$$

The last expression differs in detail for the TE and TM mode since the associated quantity α_{12} is given separately by

$$\alpha_{12} = \begin{cases} \frac{n_2 \cos \theta_2}{n_1 \cos \theta_1}, & \text{TE case;} \\ \frac{n_2 \cos \theta_1}{n_1 \cos \theta_2}, & \text{TM case.} \end{cases} \quad (4)$$

It is easily seen that $\alpha_{12}^{(\text{TE})} > \alpha_{12}^{(\text{TM})}$, for $n_2 > n_1$. Then with $\mathbb{K} = \frac{\pi}{d}$, i.e. the band edges of the first Brillouin zone, we obtain

$$\cos q_1 \cos q_2 - \Xi_{12} \sin q_1 \sin q_2 = -1. \quad (5)$$

A general characteristic of the band gaps for the TE and TM modes is that they coincide at normal incidence. The two polarization states only differ by rotational symmetry and the crystal cannot distinguish between the two. In this case, the bands are said to be degenerated. Away from the normal incident angle, the degeneracy is lifted. It is to be noted that the TE's band gaps are known to remain opened at increasing angle of incidence,¹¹ while the TM's band gaps will eventually close at certain point. This point corresponds to the Brewster's angle of TM mode. Thus, the basic constraint for an 1D ODR system is that the largest allowed incidence angle from the first (n_1) to the next layer (n_2) must satisfy the inequality, $\theta_{1(\max)} < \theta_B$, where $\theta_{1(\max)} = \arcsin \frac{n_0}{n_1}$ and $\theta_B = \arctan \frac{n_2}{n_1}$ as denoted in Fig. 1. Another common characteristic which should be taken into account is that the centers of the gaps for both the TE and TM waves are expected to shift to higher frequency at increasing angle.¹¹

These constraints determine the values of the refractive indices of the system. In terms of the gap structure, the ODR criterion is simply stated by an overlapping gaps at normal incidence and a vanishing TM's gap at grazing incident angle. In

Fig. 1. Schematic representation of the propagating light inside the one-dimensional photonic crystal with $n_0 < n_1$. The Brewster's angle θ_B inside the crystal is shown in the figure. If the difference between the background medium refractive index n_0 and that of the media is large enough, then the light will never arrive at the internal Brewster's angle.

general, the band edge of TM mode at grazing incidence angles defines the lower bound of the omnidirectional reflectance range (ω^-), while the band edge at normal incidence defines the upper bound of the omnidirectional reflectance range (ω^+). The mathematical statement of this condition is given by,

$$\omega^- = \omega_{\text{TM}}^- \left(\mathbb{K} = \frac{\pi}{d}, \theta_0 = \frac{\pi}{2} \right), \quad \omega^+ = \omega_{\text{TE,TM}}^+ \left(\mathbb{K} = \frac{\pi}{d}, \theta_0 = 0 \right). \quad (6)$$

Before considering a general periodic structure, it is useful to recall the best known system of quarter-wave-stack, where

$$n_1 d_1 = n_2 d_2 = \frac{\lambda_0}{4}. \quad (7)$$

At normal incidence, the center of the first band gap occurs at frequency

$$\omega_0 = \frac{2\pi c}{\lambda_0}. \quad (8)$$

After substituting Eqs. (7) and (8) into Eqs. (5) and (2) and performing straightforward manipulation, the band edges at normal incident for the quarter-wave-stack are given as

$$\omega^\pm = \omega_0 \left[1 \pm \frac{2}{\pi} \arcsin \left(\left| \frac{n_2 - n_1}{n_2 + n_1} \right| \right) \right]. \quad (9)$$

Note that Eqs. (2) and (7) readily yield $q_1 = q_2$ at normal incident. This further leads to the following expressions

$$q_1^\pm = q_2^\pm = \frac{\pi}{2} \pm \phi \quad (10)$$

where the phase shift ϕ is given by

$$\phi = \arcsin \left(\left| \frac{n_2 - n_1}{n_2 + n_1} \right| \right). \quad (11)$$

Thus, extending the above result for a general structure at any incident angle, we may write, following Lekner,⁸ Eq. (10) into the form

$$q_1^\pm = \frac{2D_1}{D_1 + D_2} \left(\frac{\pi}{2} \pm \phi^\pm \right), \quad (12)$$

$$q_2^\pm = \frac{2D_2}{D_1 + D_2} \left(\frac{\pi}{2} \pm \phi^\pm \right), \quad (13)$$

where the phases $\phi^\pm$ are to be found for each polarization as follows. After substituting Eqs. (12) and (13) into Eq. (5), and performing a straightforward manipulation, the transcendental equation may be converted into the form,

$$\sin \phi^\pm = A \cos \left[B \left(\frac{\pi}{2} \pm \phi^\pm \right) \right] \quad (14)$$

where

$$A = \sqrt{\frac{\Xi_{12} - 1}{\Xi_{12} + 1}} = \sqrt{\left(\frac{\alpha_{12} - 1}{\alpha_{12} + 1} \right)^2} = \left| \frac{\alpha_{12} - 1}{\alpha_{12} + 1} \right| \quad (15)$$

Fig. 2. Illustration of variation of B with respect to index contrast Δn for the case with $n_1 = 1.6$, $n_2 = n_1 + \Delta n$ and thicknesses $d_1 = 1.5 \mu m$, $d_2 = 4.5 \mu m$ on air background. The solid line represents values at normal incidence, the dotted line represents values at $\sin \theta = 0.5$ and the dashed line represents values at grazing incidence.

and

$$B = \frac{D_2 - D_1}{D_2 + D_1}.$$

The band edge frequencies can be found using Eqs. (12), (13) and (2) to yield

$$\omega^\pm = \frac{2c}{D_1 + D_2} \left(\frac{\pi}{2} \pm \phi^\pm \right). \quad (16)$$

This result automatically reduces to that of the quarter-wave-stack for normal incidence.

For many structures that have been analyzed and fabricated, $\phi^\pm$ are invariably small quantities, whereas B is **not**. This is illustrated in Fig. 2 for a wide range of index contrast Δn . Hence, different from Ref. 8, one should first expand Eq. (14) as

$$\sin \phi^\pm = A \cos \left(B \frac{\pi}{2} \right) \cos (B\phi^\pm) \mp A \sin \left(B \frac{\pi}{2} \right) \sin (B\phi^\pm). \quad (17)$$

Then taking the approximation

$$\cos (B\phi^\pm) \approx 1 - \frac{1}{2} (B\phi^\pm)^2,$$

and

$$\sin (B\phi^\pm) \approx B\phi^\pm,$$

we arrive at the expression,

$$\phi^\pm = \arcsin \left[A \cos \left(B \frac{\pi}{2} \right) - \frac{A}{2} (B\phi^\pm)^2 \cos \left(B \frac{\pi}{2} \right) \mp A (B\phi^\pm) \sin \left(B \frac{\pi}{2} \right) \right]. \quad (18)$$

In view of the smallness of $\phi^\pm$, further expansion by Taylor series of $\arcsin(x + \delta x)$ with $x = A \cos(B\frac{\pi}{2})$ and $\delta x = -\frac{A}{2}(B\phi^\pm)^2 \cos(B\frac{\pi}{2}) \mp A(B\phi^\pm) \sin(B\frac{\pi}{2})$, results in the final approximate expression to the first order in δx (second order in $\phi^\pm$),

$$\phi^\pm = \arcsin \left\{ A \cos \left(B \frac{\pi}{2} \right) \right\} - \frac{A \left\{ \frac{1}{2} \cos \left(B \frac{\pi}{2} \right) (B\phi^\pm)^2 \pm \sin \left(B \frac{\pi}{2} \right) (B\phi^\pm) \right\}}{\sqrt{1 - A^2 \cos^2 \left(B \frac{\pi}{2} \right)}}. \quad (19)$$

After regrouping terms according to different powers of $\phi^\pm$, we obtained the following quadratic relation

$$\left[\frac{AB^2 \cos \left(B \frac{\pi}{2} \right)}{2\sqrt{1 - A^2 \cos^2 \left(B \frac{\pi}{2} \right)}} \right] (\phi^\pm)^2 + \left[1 \pm \frac{AB \sin \left(B \frac{\pi}{2} \right)}{\sqrt{1 - A^2 \cos^2 \left(B \frac{\pi}{2} \right)}} \right] \phi^\pm - \arcsin \left\{ A \cos \left(B \frac{\pi}{2} \right) \right\} = 0. \quad (20)$$

Solving the above equation and selecting the positive roots give the desired expression for $\phi^\pm$. The analytic expression for the band edges $\omega^\pm$ can in turn be found by substituting expressions of $\phi^\pm$ into Eq. (16). The results of a specific case is illustrated in Fig. 3. Note that the figure also includes the results of Ref. 8 in which the cosine function of the right-hand side of Eq. (14) is expanded directly in Taylor series, leading to the following expressions for the phase shift,

$$\tilde{\phi}^\pm = \arcsin A - \frac{|\alpha_{12} - 1|}{4\sqrt{\alpha_{12}}} B^2 \left[\frac{\pi}{2} \pm \arcsin A \right]^2, \quad (21)$$

which is correct for small B only.

One readily sees the excellent agreement between the solid curves plotted on the basis of Eq. (20) and the numerical result. The dashed curves plotted according to Eq. (21) on the other hand exhibit perceptible deviations. Further, while the solid curves show widening TE gap with increasing angle θ as expected on general physical ground, the reverse is displayed by the dashed lines, implying narrowing TE gap with increasing θ . This deviation apparently stems from the inappropriate assumption of small B in general.

A comparison with the result in Ref. 8 and further verification of our result, are provided by considering the dependencies of band edges on the filling fraction $\nu = \frac{d_2}{d}$ and the index contrast. These are best described by the bifurcation diagrams presented in Figs. 4 and 5 at different incident angles for the TE band. It is immediately clear from these figures that our results agree almost perfectly with numerical results over the entire range of variations in ν as well as Δn considered for different incident angles. In contrast, the $\omega - \nu$ and $\omega - \Delta n$ curves plotted on the basis of Ref. 8 are found to deviate ostensibly from the numerical results both qualitatively and quantitatively. Almost the same features shown in Figs. 4 and 5 are found in the TM case.

Fig. 3. (a) The complete band structure for a system with $n_1 = 1.43$, $n_2 = 3.40$, $d_1 = d_2 = 90$ nm. Dots represent the numerical result. Solid curves and dashed curves show respectively the approximation based on the improved Eqs. (20) and (21) derived in Ref. 8. (b) The close-up view of the upper band edges exposing the narrowing trend of the TE gap.

Fig. 4. Bifurcation diagram of frequency ω versus filling fraction ν for the case with refractive indices $n_0 = 1.0$, $n_1 = 1.6$ and $n_2 = 4.6$. The numerical results are represented by dots. The approximated band edges for TE mode based on Eq. (20) are given respectively for (a) $\theta = 0$, (b) $\theta = \frac{\pi}{4}$ and (c) $\theta = \frac{\pi}{2}$.

3. The Band Gap

Having determined the band edges, it is straight forward to obtain the corresponding band gaps. This is illustrated for certain refractive indices in Fig. 6, where the bifurcation diagrams for normal incidence and grazing incidence of TM wave are plotted with respect to the filling fraction. The omnidirectional band gap, which is an overlapping part of the two adjacent gaps is shown as shaded area for the lower order band gap.

As pointed out in Ref. 8, the approximated analytical expressions of the band edges allow us to determine the minimum condition for the occurrence of omnidirectional reflection. A dimensionless parameter used to quantify the extent of the

Fig. 5. Variation of upper and lower band edges with respect to changes in index contrast for system with $n_1 = 1.6$, $n_2 = n_1 + \Delta n$ and thicknesses $d_1 = 1.5 \mu m$, $d_2 = 4.5 \mu m$. The numerical results are represented by dots. The approximated band edges for TE mode based on Eq. (20) are given respectively for (a) $\theta = 0$, (b) $\theta = \frac{\pi}{4}$ and (c) $\theta = \frac{\pi}{2}$.

omnidirectional range is the **relative bandwidth** ξ defined as

$$\xi = \frac{\Delta\omega}{\langle\omega\rangle} = \frac{\omega^+ - \omega^-}{\frac{1}{2}(\omega^+ + \omega^-)}. \quad (22)$$

Here $\Delta\omega$ is the width of the omnidirectional reflection band and $\langle\omega\rangle$ is the mid-gap frequency. The quantity ξ can be further expressed in terms of the system parameters. Obviously, the omnidirectional range is bounded by $\xi \geq 0$.

In order to see the implications of this lowest bound of ξ on the refractive indices, we have plotted on Fig. 7 the contour of equi-omnidirectional lines, i.e. lines with

Fig. 6. The bifurcation diagram of the filling fraction for a system with $n_0 = 1.00$, $n_1 = 1.43$ and $n_2 = 4.60$, ω is normalized to $\frac{2\pi c}{d}$. The solid (dashed) curves are the band edges for normal (grazing-angle) incidence. The shaded area indicates the first omnidirectional band gap. The inset shows the relative bandwidth ξ , defined by Eq. (22), plotted versus the filling fraction ν .

Fig. 7. Contours of equi-omnidirectional lines on $(\delta n_1, \delta n_2)$ plane showing the extreme point of n_2 , ($\delta n_1 = 1.492045$, $\delta n_2 = 2.246763$). The optimal thickness ratio of this extreme point is $\rho = 1.362086$.

constant ξ , on the $(\delta n_1, \delta n_2)$ plane, where $\delta n_2 = \frac{n_2}{n_0}$ and $\delta n_1 = \frac{n_1}{n_0}$. It is seen from the figure, that there is a clear minimum of n_2 on each equi-omnidirectional line. This extreme point of n_2 correspond to $\xi = 0$ and gives the minimum value of the high refractive index. Stated differently, we have for this case $\omega^+ = \omega^-$, or using the defining equations for ω^+ and ω^- , Eqs. (14) and (16), we have

$$\beta = \frac{\frac{\pi}{2} + \phi^+}{1 + \rho} = \frac{\frac{\pi}{2} - \phi^-}{r_1 + \rho r_2} \quad (23)$$

where $\rho = \frac{n_2 d_2}{n_1 d_1}$ is the optical path ratio, which reduces to 1 for the quarter-wave stack and $r_j = \sqrt{1 - (\frac{n_0}{n_j})^2}$ for $j = 1, 2$.

Inserting the appropriate ϕ^+ and ϕ^- as found from the quadratic Eq. (20), we can find numerically the minimum condition for the existence of ODR. The resulted values are as follows,

$$\begin{aligned} n_2 &= 2.24676339n_0, \\ n_1 &= 1.4920n_0, \\ \rho &= 1.3621. \end{aligned} \quad (24)$$

The values obtained using the approximate Eq. (21) are⁸

$$\begin{aligned} n_2 &= 2.247n_0, \\ n_1 &= 1.493n_0, \\ \rho &= 1.352. \end{aligned} \quad (25)$$

Obviously our result is closer to the exact result given in Ref. 8 as listed below:

$$\begin{aligned} n_2 &= 2.246763n_0, \\ n_1 &= 1.492045n_0, \\ \rho &= 1.362086. \end{aligned} \quad (26)$$

4. Parameters Optimization

Figure 6 reveals that there is a clear maximum of bandwidth. As one of the most important parameters characterizing the performance of an ODR, the relative bandwidth ξ introduced by Eq. (22) is naturally the quantity to be optimized in the system design. To this end, an analytic formulation would be highly desirable. We shall show in the following that this can be done for the case with a given set of refractive indices. In this case, ξ becomes a function of the single parameter ν , and can be written with the help of Eq. (16) in the following form,

$$\xi(\nu) = 2 \frac{\beta_2(\nu) - \beta_1(\nu)}{\beta_2(\nu) + \beta_1(\nu)} \quad (27)$$

where

$$\beta_1 = \frac{\frac{\pi}{2} + \phi^+(\nu)}{1 + \rho}, \quad \beta_2 = \frac{\frac{\pi}{2} - \phi^-(\nu)}{r_1 + \rho r_2}. \quad (28)$$

Optimization of $\xi(\nu)$ with respect to ν simply implies

$$\frac{d\xi(\nu)}{d\nu} = 4 \frac{\frac{d\beta_2(\nu)}{d\nu} \beta_1(\nu) - \frac{d\beta_1(\nu)}{d\nu} \beta_2(\nu)}{(\beta_2(\nu) + \beta_1(\nu))^2} = 0 \quad (29)$$

which yields the following relation

$$\frac{\frac{d\beta_2(\nu)}{d\nu}}{\frac{d\beta_1(\nu)}{d\nu}} = \frac{\beta_2}{\beta_1}. \quad (30)$$

Meanwhile, using Eq. (28), Eq. (14) can be rewritten as

$$f(\nu, \beta_2) = \tan(\rho\beta_2) \tan(\beta_2) - \frac{n_2}{n_1} = 0, \quad (31a)$$

$$g(\nu, \beta_1) = \tan(\rho r_2 \beta_1) \tan(r_1 \beta_1) - \frac{n_1 r_2}{n_2 r_1} = 0. \quad (31b)$$

Differentiating $f(\nu, \beta_2)$ and $g(\nu, \beta_1)$ with respect to ν gives

$$\frac{\partial f}{\partial \nu} + \frac{\partial f}{\partial \beta_2} \frac{d\beta_2}{d\nu} = 0, \quad (32a)$$

$$\frac{\partial g}{\partial \nu} + \frac{\partial g}{\partial \beta_1} \frac{d\beta_1}{d\nu} = 0. \quad (32b)$$

The factors $\frac{d\beta_1}{d\nu}$ and $\frac{d\beta_2}{d\nu}$ in these equations can be eliminated by means of Eq. (30), resulting in the following equation

$$h(\nu, \beta_1, \beta_2) = \frac{\frac{\partial f}{\partial \nu}}{\frac{\partial g}{\partial \nu}} - \frac{\frac{\partial f}{\partial \beta_2} \beta_2}{\frac{\partial g}{\partial \beta_1} \beta_1} = 0. \quad (33)$$

We thus have 3 equations: (31a), (31b) and (33), and 3 unknowns: ν , β_1 and β_2 , which are solvable. However, these equations, being transcendental equations, can only be solved numerically. For a system with $n_1 = 1.43$ and $n_2 = 4.60$ as depicted in the inset in Fig. 6, we find that $\nu = 0.252950$ which correspond to $\xi = 43.03\%$. Had one used the system parameters of $n_1 = 1.40$ and $n_2 = 3.40$, the optimized filling fraction would be $\nu = 0.324652$ corresponding to a relative bandwidth of $\xi = 25.02\%$. This optimized value of the relative bandwidth of an ODR is in good agreement with the numerical result reported in Ref. 5.

5. Conclusion

We have presented the result of analysis of the band edge structure of the 1D omnidirectional reflector. By extending the first order results of Ref. 8 to second order approximation, we have achieved a more consistent result and much better agreement with numerical results. We have also established the minimum refractive indices required by the ODR operation in both TE and TM modes, which turns out to be the same as given in Ref. 8.

Further, a semi-numerical scheme has been developed on the basis of our approximate band edge formulation for the optimization of the relative bandwidth

with respect to the filling fraction. This allows the determination of the maximum band gap by a proper choice of the thicknesses of the dielectric layers for a given refractive indices. Application of this scheme to specific example testifies to the accuracy of our formulation.

Acknowledgments

This work is supported by the RUTI project no. 149B-11/SK/RUTI/2002 of the State Ministry of Research and Technology and the Hibah Bersaing XI project of the Ministry of National Education of the Republic of Indonesia. The support of the Royal Dutch Academy of Science and Arts (KNAW) through the Extended Programme Applied Mathematics (EPAM) Project is gratefully acknowledged.

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