Extremal characterization of band gaps in nonlinear gratings

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Abstract
In this paper we present an explicit extremal characterization of the edges of the lowest band gap in gratings; we restrict here to the case of TE-modes, but the TM case can be treated similarly.
The characterization is valid for linear and Kerr-nonlinear gratings, for smooth as well as for step-variations of the index and the coefficient of nonlinearity. The variational characterization allows one to derive monotonicity properties by using simple comparison arguments. For instance, the monotonic shift of the band gap as a function of the angle of oblique incidence is proved, leading to a simple criterion for omni-directionally for the band gap. Rough estimates of the band gaps can be obtained by substituting suitable trial fields in the governing functionals, while the same formulation can also be used to design a Finite Element scheme for accurate calculations.

1 Introduction
In this paper we will characterize for 1D gratings the precise values of the edges of the band gaps. To simplify the notation and reduce the number of formulae, we will only consider the lowest band gap. Furthermore, we will restrict to TE-modes, remarking that TM-modes can be studied similarly. On the other hand, we will allow arbitrary (periodic) index profiles and third order nonlinearity with spatial dependent (periodic) coefficient. Then for time harmonic fields, and normal incidence, the governing equation for the spatially dependent amplitude $E$ reads
$$\partial_z^2 E + \omega^2 [n^2(z) + \gamma(z)|E|^2] E = 0.$$ (1)
Here $\omega$ is the normalized frequency (the velocity of light has been normalized to unity), $n(z), \gamma(z)$ are the index of refraction and the coefficient of nonlinearity respectively. Special cases such as step-wise index variations and linear gratings are included. The period will be denoted by $p$ in the following.

Studying (1) for varying $\omega$ leads to (nonlinear variants of) Bragg dispersion outside the band gap, and full reflection inside the band gaps. In this paper we will characterize the edges of the first band gap by giving a variational (extremal) characterization for the corresponding values of $\omega$, i.e. we will deal with (1) as a (nonlinear) eigenvalue problem.
The extremal formulation will make it possible to study the dependence of the position of the band gap on the physical parameters $n, \gamma$, and will make it possible to find estimates for the band gap by comparison with simpler structures. For instance, for oblique incidence from a uniform half-space with index $n_0$ under an angle $\theta$, in which case the governing equation is
$$\partial_z^2 E + \omega^2 [(n^2(z) - n_0^2 \sin^2 \theta) + \gamma(z)|E|^2] E = 0,$$ (2)
the extremal characterization will immediately give the result that the band gap shifts monotonically. By its nature, the extremal characterization can also be applied to obtain numerical approximations for

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2 Extremal characterization at normal incidence

2.1 Shift-skew symmetry of Edge states

For linear, infinitely long gratings the first band gap is the smallest interval of frequencies for which there is total reflection. Reviewing Floquet’s (Bloch’s) theorem, this happens at the end of the first Brillouin zone which consists of solutions that modulate a $p$-periodic function with a $z$-harmonic modulation $E = v(z)e^{iK(\omega)z}$; in the band gap, the ‘wave number’ $K(\omega)$ is complex, with $\text{Re}(K(\omega)) = \pi/p$ and the imaginary part is the exponential growth (decay) of the solution inside the band gap. At the edge of the band gap, $\text{Im}(K(\omega)) = 0$, and the solution is of the form $E = v(z)e^{i\pi z/p}$. This shows that the edge states satisfy

$$E(z + p) = -E(z)$$

which we will call ‘shift-skew (ss)-symmetric’; of course this implies these states are $2p$-periodic. The edges of the band gap are the values of $\omega$ for which such a ss-symmetric solution exists. This shows that we consider (1) as a (nonlinear) eigenvalue problem for the set of ss-symmetric functions. We can reduce this problem to a problem on an interval of one period by observing that the edge states vanish at some point, say at $z = \xi$:

$$E(\xi) = E(\xi + p) = 0,$$

which at first sight reduces the problem to a simple Dirichlet boundary value problem (DBVP). However, the precise position of the interval is not known in advance, i.e. $\xi$ is unknown. Having a solution on the specified interval, a smooth, i.e. differentiable, ss-symmetric continuation is possible only if the derivatives at the endpoints are related according to:

$$\partial_z E(\xi) = -\partial_z E(\xi + p).$$

This additional condition should be added to the DBVP. An arbitrary choice of $\xi$ will not lead to a solution that satisfies this condition, but in the following we will see that for suitable $\xi$ this condition can be satisfied.

2.2 Variational formulation

The linear DBVP, $\gamma = 0$, is a standard linear eigenvalue problem for which eigenvalues $\omega^2$ and eigenfunctions can be found in a well known variational way as the critical values and points of the Rayleigh quotient. Briefly, if $u$ is a critical point of the quotient $R(u) = Q(u)/N_{\text{lin}}(u)$, where

$$Q(u) = \int_\xi^{\xi+p} (\partial_z u)^2 dz, \quad N_{\text{lin}}(u) = \int_\xi^{\xi+p} n^2(z)u^2 dz,$$

and satisfies the Dirichlet conditions, then $u$ satisfies (1) with $\omega^2$ given by the value of this quotient at the solution. The quadratic homogenity of the functionals implies that any of the functionals can be taken as constraint for variations of the other functional; the constraint prescribes the norm of the solution to be found. For the linear problem, the value of the constraint is irrelevant, but it is the constrained formulation that can be generalized to the nonlinear problem, in contrast to the
formulation with the Rayleigh quotient. This generalization will now be described.

To include the nonlinearity, define the functional

\[ N(u) = \int_{\xi}^{\xi+p} \left[ n^2(z)u^2 + \frac{1}{2} \gamma(z)u^4 \right] dz \]

and consider the constrained maximization problem

\[ \max_u \{ N_\xi(u) \mid Q(u) = A, \; u(\xi) = u(\xi + p) = 0 \} . \]

Then, Lagrange’s multiplier rule applies and states that for some multiplier \( \lambda \) the maximizer \( U \) satisfies the Euler Lagrange equation

\[ n^2U + \gamma U^3 = -\lambda \partial^2_z U, \]

the constraint condition, and the Dirichlet boundary conditions. Provided \( \lambda \) is positive, for \( \omega^2 = 1/\lambda \) this is precisely (1). By multiplying this equation by \( U \), and integrating over the interval, shows that \( \lambda \) is given by \( \lambda = \int \left[ n^2U^2 + \gamma U^4 \right] / Q(U) \); for positive \( \gamma \) this is positive, but it is also positive for negative \( \gamma \) provided the nonlinearity is not too large.

The maximizer \( U \) found in this way is not yet an acceptable field distribution \( E \) since the additional boundary condition still has to be satisfied. And, preferably, a more explicit characterization of the multiplier. To that end, we investigate the dependence of the value of the minimization problem on the position of the interval and the value of the constraint:

\[ V(A, \xi) = \max_u \{ N(u) \mid Q(u) = A, \; u(\xi) = u(\xi + p) = 0 \} \]

and denote for given \( \xi \) the maximizing solution by \( U \) and the multiplier by \( \lambda \). Then we have both desired results as follows.

**Claim 1** For any \( \xi \), the multiplier is the derivative with respect to the constraint of the value function:

\[ \lambda = \frac{d}{dA} V(A, \xi). \]

For given \( A \), let \( \xi \) be a critical point of the value function \( V(A, \xi) : \partial_\xi V(A, \xi) = 0 \). Then the solution \( U(\xi) \) satisfies the additional boundary condition and is an actual physical field distribution \( E \).

The proof of the claims is based on standard reasoning from the Calculus of Variations and will therefore not be given here.

Of course, at fixed \( A \), the value function over one period has a maximum and a minimum value, at which points the required additional boundary condition will be satisfied; the corresponding solutions and multipliers will correspond to the edges of the band gap. Based on this, we can now finish this section with a summary. At the same time we make a simplification of the notation which is handy for the following. First it is convenient to transform to a problem on a fixed interval and to replace the shift of the interval by a shift of the inhomogeneous terms in the functionals. Taking \([0, p] \) as the interval, the functionals are then given by

\[ Q(u) = \int_0^p (\partial_z u)^2 \; dz, \quad N_\xi(u) = \int_0^p \left[ n^2(z + \xi)u^2 + \frac{1}{2} \gamma(z + \xi)u^4 \right] dz. \]
The formulae for the lower and the upper edge of the band gap are then

\[
\left( \frac{\omega^2}{\Omega^2} \right) (A) = \left( \frac{\max_n}{\min_n} \right) \frac{d}{dA} V(A, \xi),
\]

with

\[
V(A, \xi) := \max_u \{ N_\xi(u) \mid Q(u) = A, \ u(0) = u(p) = 0 \}.
\]

Note that for linear gratings, with \( \gamma = 0 \), the value function is linear in the constraint \( A \) and the differentiation to find the multiplier can be avoided by normalizing \( A = 1 \).

For nonlinear gratings a similar simplification can be achieved as follows. In fact, exploiting the fact that we are dealing with integrands in the functionals that are just polynomials, and in particular that the functional \( Q \) is quadratic, the value of the constraint can be normalized, leading to

\[
V(A, \xi) := \max_u \{ N_{\xi, A}(u) \mid Q(u) = 1, \ u(0) = u(p) = 0 \}; \tag{3}
\]

with

\[
N_{\xi, A}(u) = \int_0^p An^2(z + \xi)u^2 + \frac{1}{2} A^2 \gamma(z + \xi)u^4 \, dz \tag{4}
\]

This is the final formulation, valid for linear and nonlinear gratings, that will be used in numerical calculations in the following.

**Remark 2** For step-gratings, with steps at \( z_{\text{step}} \), note that \( \partial_n n^2(z + \xi) = \sum_{\text{steps}} [\pm \delta_{\text{Dirac}}(z - z_{\text{step}})] \), with plus or minus sign for a positive, resp. negative step. From this it follows that in a two-step grating, the values of the field at each side of a layer are either the same or opposite. The field at the lower edge is the same at the edges of the high-index material, while the field at the upper edge of the band gap is the same at the edges of the low-index region. For gratings that also have stepwise changes in the nonlinearity, additional symmetry conditions arise.

### 3 Oblique incidence and omni-directional band gap

An immediate consequence of the extremizing formulation above is the possibility to derive inequalities. For instance, if for the same \( \gamma \), the index is changed, say decreases at each point, for each trial function \( u \), and each \( \xi \), the functional \( N_{\xi, A}(u) \) will decrease, while \( Q(u) \) remains unaltered, leading to a decrease of \( \frac{d}{dA} V(A, \xi) \), and then a decrease of both \( \max_\xi \frac{d}{dA} V(A, \xi) \) and \( \min_\xi \frac{d}{dA} V(A, \xi) \). which will correspond to an increase of the values for the band gap. We will now exploit this to investigate the omni-directionality of the band gap.

An omni-directional band gap is a range of frequency \( \omega \) such that under all incident angle \( \theta \in [0, \pi/2) \) there are no propagating solutions for (2), or total reflection. The existence of omni-directional band gap in periodic structures has also been discussed in several publications\(^2\)\(^-\)\(^5\) using the transfer matrix approach. Here we use extremal characterization which will give the possibility for direct calculation of the band gap edges for arbitrary periodic index profile.

#### 3.1 Monotonicity for oblique incidence

For oblique incidence to a linear grating (\( \gamma = 0 \)), the index of refraction in the governing equation and in the functional \( N_{\xi, A}(u) \) is replaced by the effective index \( n^2 - n_0^2 \sin^2(\theta) \) with \( \theta \) the angle with the normal. Hence the index decreases monotonically with increasing \( \theta \in [0, \pi/2) \) to a lowest value \( n^2 - n_0^2 \) at grazing incidence. Assuming \( n^2 - n_0^2 \) to be positive, the above reasoning applies and we conclude that both band gap edges \( \omega(\theta) \) and \( \Omega(\theta) \) are monotonically increasing functions of \( \theta \). Examples are
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(a) Parameters: $n_0 = 1$, $n_a = 1.544 \rightarrow \text{SiO}_2$, $n_L = 2.616 \rightarrow \text{TiO}_2$, and the width of each cell: $a = b = \pi/2$.

(b) Parameters: $n_0 = 1$, $n_a = 2.354 \rightarrow \text{ZnS}$, $n_L = 2.616 \rightarrow \text{TiO}_2$, and the width of each cell: $a = b = \pi/2$.

Figure 1: Examples of band gap edges from structure with omni-directional band gap (a), and without omni-directional band gap (b). Parameters for these (half infinite) linear grating with step-wise varying index are as indicated above.

given in Figures 1.a and 1.b for a linear grating with step-wise varying index. Figure 2 shows the same pattern for a harmonic change of the index; this case cannot be solved explicitly and the plot has been produced using the numerical method to be explained below.

Figure 2: Band gap edges for (half infinite) linear grating with harmonic index profile $n(z) = \bar{n}(1 + \varepsilon \cos(z))$. Here $\bar{n} = 1.923 \rightarrow \text{ZrSiO}_4$, and $\varepsilon = 0.2$.

For a linear grating the value function is linear in the constraint $A$, and has nonzero derivative for each $A$. For small nonlinearity, the monotonicity in $\theta$ will therefore not be disturbed; an example is shown in Figure 3.
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Figure 3: Band gap edges for (half infinite) nonlinear grating with step-wise varying index. Parameters: \( n_0 = 1, n_a = 1.544 \rightarrow \text{SiO}_2, n_b = 2.616 \rightarrow \text{TiO}_2 \), and the width of each cell: \( a = b = \pi/2 \). Furthermore \( \gamma = 0.2 \) and \( A = 1 \).

3.2 Omni-directional band gap

Omni-directional reflectance will be present when the lower edge at grazing incidence is smaller than the upper edge value at normal incidence

\[ \omega(\pi/2) < \Omega(0) \]

A sufficient condition could be obtained from an upperbound for \( \omega(\pi/2) \) and a lowerbound for \( \Omega(0) \). An upperbound for \( \omega(\pi/2) \) has been constructed above. A lowerbound for \( \Omega(0) \) can be obtained from the saddle point character: in each neighbourhood there are functions with a lower value. Explicit functions can be found as follows. Suppose \( U_\zeta(z) \) is the solution of

\[ U_\zeta(z) \in \min_{\zeta} \frac{d}{dA} V(A, \xi) \]

which reaches the minimal value at \( \bar{\zeta} \):

\[ \Omega^{-2}(0) = N_{\bar{\zeta}, A}(U_\bar{\zeta}, 0) \]

Then a lower value is attained for each \( U_\zeta \) with \( \zeta \) close to \( \bar{\zeta} \). In a numerical procedure that searches for this minimum, such functions will be easily found.

4 Approximate and numerical results

In the previous section we have shown the applicability of the extremal characterization to obtain monotonicity properties about the dependence on the angle of incidence. Now we show that as

\[ \text{More fundamentally, it can be found by observing that it is a function in the tangent direction: } U_\zeta + \epsilon W \text{ with } W = \partial_\zeta U_\zeta(z)|_{\zeta=\bar{\zeta}} . \]

For linear gratings, \( W \) satisfies the same equation (but with different boundary conditions: \( W(\bar{\zeta}) = -W(\bar{\zeta} + p) \neq 0 \)). Hence it is the solution adjoint to \( U_\zeta \) that can be expressed in a standard way for second order equations, explicitly:

\[ W(z) = U_\zeta(z) \int^z dz' \frac{dz'}{U_\zeta(z')^2} \]

Hence, having found an approximation for \( U_\zeta(z) \) an approximation for \( W \) can thus be derived and a shift in this direction will produce a lower bound, provided the approximation is sufficiently accurate.

For nonlinear gratings, \( W \) will satisfy the linearized equation and a similar reasoning applies.
another consequence of the formulation we can derive simple approximations for the band gap, or, alternatively, design a simple FEM code with which accurate calculations can be performed.

4.1 Approximate field functions

Just as the minimum value of a function can be estimated above by its value at any point, we can take an ‘arbitrary’ function (or a parameterized family of trial functions) in the variational formulation and find bounds for the value function and then the band gap edge. Of course, the accuracy of the bound depends on the choice of the trial function.

To show this in some detail, for instance to approximate the lower edge, take a function \( W \) that satisfies the Dirichlet boundary conditions and then find the optimal value of the index-shift. With the normalization \( Q(W) = 1 \), for each \( \xi \)

\[
V(A, \xi) := \max_u \{ N_{\xi,A}(u) \mid Q(u) = 1, \} \geq N_{\xi,A}(W)
\]

and hence \( \max_\xi V(A, \xi) \geq N_{\xi,A}(W) \) and then

\[
\max_\xi V(A, \xi) \geq \max_\xi N_{\xi,A}(W)
\]

For a linear problem (take \( A = 1 \)) this implies we have an immediate upperbound for the lower edge:

\[
\omega^{-2} \geq \max_\xi N_{\xi,A}(W)
\]

and similarly for the upper edge for a trial function \( V \):

\[
\Omega^{-2} \geq \min_\xi N_{\xi,A}(V).
\]

with rhs that can be computed directly.

With respect to the quality of the upperbound depending on the choice of \( W \) and \( V \), it should be noted that ‘first order’ accuracy of the field will lead to second accuracy in the determination of the critical values, owing to the fact that the first order terms vanish because of the critical point property.

Below in Figure 4 we show the resulting graphs for the choice \( W(z) = V(z) = \sin(z\pi/p) \) for each \( \theta \); this function is known to be exact when there is no index variation, and hence can be expected to be accurate for shallow gratings.

For nonlinear gratings, as an example, we calculate the band gap edges using the trial function \( W(z) \) as above, \( p = \pi \).

\[
\left( \begin{array}{c}
\omega^{-2} \\
\Omega^{-2}
\end{array} \right) (A) = \left( \begin{array}{c}
\max_\xi \\
\min_\xi
\end{array} \right) \frac{d}{dA} N_{\xi,A}(W)
\]

\[
= \left( \begin{array}{c}
\max_\xi \\
\min_\xi
\end{array} \right) \int_0^\pi \left( n^2(z + \xi) - n_0^2 \sin^2(\theta) \right) \sin^2 z \, dz + A\gamma \int_0^\pi \sin^4 z \, dz
\]

Evaluating the integral above results in an explicit function of \( \xi \) for the band gap edges

\[
\left( \begin{array}{c}
\omega^{-2} \\
\Omega^{-2}
\end{array} \right) (A) = \left( \begin{array}{c}
\max_\xi \\
\min_\xi
\end{array} \right) \frac{1}{2} \left( n_1^2 - n_0^2 \right) \sin(2\xi) + \frac{\pi}{4} (n_1^2 + n_0^2) - \frac{\pi}{2} n_0^2 \sin^2 \theta + A\gamma \frac{3\pi}{8}
\]

Clearly, \( \omega^{-2} \) and \( \Omega^{-2} \) is obtained if \( \xi = \pi/4 \) and \( \xi = 3\pi/4 \) respectively. We show the resulting band gap edges in Figure 6.a for various values of \( \gamma \).
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Figure 4: Band gap edges approximation using trial function $W(z) = \sin(z\pi/p)$ (solid line) as indicated above and the exact result (dashed line), for (half infinite) linear grating with step-wise varying index. Parameters: $n_0 = 1$, $n_a = 1.544 \rightarrow \text{SiO}_2$, $n_b = 2.616 \rightarrow \text{TiO}_2$, and the width of each cell: $a = b = \pi/2$.

4.2 FEM calculations

Above we took a simple harmonic function as trial function. Another way, to obtain more accurate results, is to approximate a function as a superposition of base function, and optimize with respect to the choice of the expansion coefficients. If the base functions are taken to be local spline functions this leads to the Finite Element Method. We will now briefly describe this. For a given grid, $(z_0, z_1, \ldots, z_N, z_{N+1})$, with $z_0 = 0$, $z_{N+1} = p$, take piecewise linear base functions: $\varphi_m$ with $\varphi_m(z_m) = 1$, and vanishing at other grid points. For a given function write $u(z) = \sum_{m=1}^{N} u_m \varphi_m(z) \equiv \vec{u} \cdot \vec{\varphi}(z)$ with $u_m = u(z_m)$. Then ‘discretize’ the functionals by restriction to such expansions, obtaining functions of $\vec{u}$:

$$\hat{Q}(\vec{u}) := Q(\vec{u} \cdot \vec{\varphi}(z)), \quad \hat{N}_{\xi,A}(\vec{u}) := N_{\xi,A}(\vec{u} \cdot \vec{\varphi}(z))$$

The corresponding extremal problem then leads, for fixed $\xi$, to the Euler Lagrange equation for $\vec{u}$:

$$\nabla \hat{N}_{\xi,A}(\vec{u}) = \mu \nabla \hat{Q}(\vec{u}),$$

where $\nabla$ consists of differentiation with respect to the vector $\vec{u}$. In more detail, the equation contains matrices $F_\xi$, $G$ and a matrix $R(\vec{u})$ depending quadratically on $\vec{u}$ such that

$$[AF_\xi + A^2R(\vec{u})] \vec{u} = \mu G\vec{u}.$$  

For linear problems, $R = 0$, this is a standard eigenvalue problem, for which the largest eigenvalue is sought, say $\mu(\xi)$. Then $\max_\xi \mu(\xi)$ leads to an approximation for the lower edge, and $\min_\xi \mu(\xi)$ for the upper edge of the band gap.

When the problem is nonlinear, an iteration method is required to deal with the nonlinearity; a simple way is to take the nonlinear term at a previous iterate:

$$[AF_\xi + A^2R(\vec{u}(j))] \vec{u}^{(j+1)} = \mu^{(j+1)} G\vec{u}^{(j+1)}, \quad Q(u^{(j+1)}) = 1.$$  

When converged, the computed largest eigenvalue $\mu(\xi)$ gives the value function $V(A, \xi)$ for a fixed value of $A$. Then a central difference scheme is used to calculate the derivative of the value function, which leads just as above to the approximations of the lower and upper edge.
The method described above is second order accurate, say FEM2. When taking a uniform mesh, with an even number of points, a simple method known as Richardson extrapolation can be used to arrive at a fourth order scheme: FEM4. We have used this method to obtain the previous figures when no exact solution was possible.

Below we show the performance in a linear case with step-index for which the exact band gap can be calculated with matrix transfer technique: in Figure 5.a and 5.b we present the error for the lower edge of the band gap, defined as

\[
\text{error} = \frac{|\omega_{\text{app}} - \omega_{\text{exact}}|}{\omega_{\text{exact}}}
\]

for three different methods: the trial function \(\sin(\pi z/p)\), FEM2 and FEM4 for 16 and 32 elements.

In Figure 6.a and 6.b, the results for a nonlinear grating with a trial function and FEM4 are shown. The finite elements calculations were implemented using MATLAB. Each set of computations, such as the graphs in Figure 6 takes less than two seconds on a regular PC.

5 Conclusion and remarks

In this paper we have characterized the edges of the first band gap in a variational way. Essential for that is that we can use the fact that the corresponding fields vanish at the end points of an interval of length equal to the period of the grating. Would the interval have been known in advance, a standard eigenvalue problem, extended to nonlinear case, would have resulted. Since the fields have to be extendable to 2p-periodic skew-symmetric fields, the interval had to be chosen appropriately, which could also be formulated in a variational way. For the lower-edge a double maximization formulation resulted, while for the upper-edge a mini-max formulation makes the saddle point character explicit.

This can be interpreted that the sine and cosine solutions of the Helmholtz equation that exist when the index is constant and the gap is closed, bifurcate into the two branches parameterized by the index difference.
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Simple comparison arguments were used to show that the extremal characterizations lead to the conclusion that the band gaps shift monotonically with increasing angle of incidence.

The extremal characterization makes it possible to express the value of the band gap without the necessity to calculate the edge fields in all details. Taking simple trial functions for the fields at the edges, good predictions of the band gap were found, both for linear and nonlinear gratings. For more accurate quantitative results, a numerical calculation scheme based on the FEM was designed and showed good results, fourth order of accuracy when Richardson extrapolation was applied.

The FE-scheme is used here for the approximate solution of the (nonlinear) eigenvalue problem; a comparable scheme has been used in Ref. 7 to calculate the transmittance properties, and to study the bi-stability near band gap edges, for a grating of finite length (without and with defects; see also the references in that paper to relevant literature). This problem can also be studied qualitatively by using variational methods as will be shown in a forthcoming paper. An extension of the methods of this paper to more space dimensions seems also possible, in particular for planar photonic periodic structures.

**References**


