INVITED PAPER Special Section on Photonic Crystals and Their Device Applications

# **Inverse Problem Techniques for the Design of Photonic Crystals**

# Martin BURGER<sup>†a)</sup>, Stanley J. OSHER<sup>††</sup>, and Eli YABLONOVITCH<sup>†††</sup>, Nonmembers

**SUMMARY** This paper provides a review on the optimal design of photonic bandgap structures by inverse problem techniques. An overview of inverse problems techniques is given, with a special focus on topology design methods. A review of first applications of inverse problems techniques to photonic bandgap structures and waveguides is given, as well as some model problems, which provide a deeper insight into the structure of the optimal design problems.

key words: inverse problems, optimal design, photonic crystals, wave problems, Maxwell equations, helmholtz equations

## 1. Introduction

A new paradigm has emerged, in which the band structure concepts of solid state physics are applied (cf. [1], [2]) to Electromagnetics. This has led to a profusion of scientific creativity as new forms of electromagnetic crystal structures are invented for radio and microwaves as well as for optical wavelengths. These new structures are inspired by the 3-D geometry of both natural crystals, and those artificial crystals that can arise only in the human imagination.

These artificial electromagnetic crystals (also known as photonic crystals), are impacting the diverse domains of electromagnetics, extending from radio waves to optical wavelengths. They are bringing together, under a common umbrella, scientists in the fields of Classical Electromagnetics, Solid State Band theory, semiconductor device Physics, Quantum Optics, Nano-structures, Materials Science, and now Applied Mathematics.

Essentially this field has concerned itself with artificial engineering of 3-D structures that achieve a certain goal, like a photonic bandgap. This is a design problem, but there is no direct route from the desired goal, to the structure that achieves that goal. Modern developments in formal inverse algorithms, combined with continual increases in computational power, are now replacing intuitive engineering for problem after problem. Undoubtedly the design problem of creating useful photonic bandgap structures will soon replace intuitive inspiration.

The recent development in the field of photonic crystals

Manuscript received July 15, 2003.

a) E-mail: martin.burger@jku.at

(cf. e.g. [3]–[5]) also raised several mathematical problems, such as analysis (cf. [6] for an overview), numerical simulation (cf. [3], [7], [8]), and - ultimately - design and optimization, which is the topic of this review.

### 2. Inverse Problems Techniques

In this section we shall introduce the basic concepts of inverse problems, such as the problem formulation and regularization techniques. Moreover, we shall discuss several different possibilities to model design variables, in particular the cases important for applications to photonic crystals. Finally, we discuss some optimization techniques that can be used to solve the regularized problems.

# 2.1 Problem Formulation and Regularization

In general, an *inverse problem* consists in the reconstruction or optimal design of a variable or parameter in a system in order to fit an observed or to achieve a desired state of the system. Such problems are called inverse problems, since there is an associated *direct problem*, which consists in solving (or rather simulating in engineering applications) given the value of the design variable or parameter. This direct problem is of importance for itself, but also for the solution of the inverse problem. As we shall see below any algorithm for solving the inverse problem will need solves of the direct problem with given parameters or at least solves of a linearized direct problem.

For eigenvalue problems, such as applications to photonic crystals, we usually have to deal with a problem of the form

$$U(\Lambda, U; q) \to \min_{\Lambda, U, q}$$
 (1)

subject to a state equation of the form

$$A(u_j;q) = \lambda_j B(u_j;q), \qquad j = 1, \dots, k.$$

Here,  $\Lambda = (\lambda_1, ..., \lambda_k)$  formally denotes a part of the spectrum of the direct operator,  $U = (u_1, ..., u_k)$  the vector of associated eigenfunctions, and q is the design variable. In general, one can assume that Eq. (2) is uniquely solvable for  $u_j$  and  $\lambda_j$  once the value of q is known. In order to illustrate this abstract framework, we consider a simple model problem of maximizing an eigenvalue  $\lambda_k$  of the Helmholtz equation. Since one cannot directly compute the k-th eigenvalue, we have to rewrite the problem in terms of the eigenvalues

Manuscript revised September 23, 2003.

<sup>&</sup>lt;sup>†</sup>The author is with the Department of Mathematics, UCLA, USA. On leave from Industrial Mathematics Institute, Johannes Kepler University, Linz, Austria.

<sup>&</sup>lt;sup>††</sup>The author is with the Department of Mathematics, UCLA, USA.

<sup>&</sup>lt;sup>†††</sup>The author is with the Department of Electrical Engineering, UCLA, USA.

A, the associated eigenfunctions U, and the density  $\rho$ . The functional J is then simply given by

$$J(\Lambda, U; q) = -\lambda_k = -\Lambda . e_k,$$

where  $e_k = (0, ..., 0, 1)$ . The state equation is defined by the eigenvalue problem

$$-\Delta u_j(x) = \lambda_j q(x) u_j(x), \qquad j = 1, \dots, k,$$

i.e.,

$$A(u;q) = -\Delta u, \qquad B(u;q) = qu.$$

We assume that A and B are linear and symmetric (respectively Hermitian) with respect to the state U, which is the case for the Helmholtz equation and for the Maxwell equations.

A common characteristic of most inverse problems is their *ill-posedness*, which means that the solution might not exist, might not be unique or might not depend on the data in stable way. For design problems, nonuniqueness does not create difficulties, since it is rather desirable if one can achieve a goal with different designs. Nonexistence and instability with respect to data are more serious issues for optimal design problems. A consequence of unstable dependence on the data is that for arbitrarily small changes of parameters in the system arbitrarily large differences in the optimal design can occur, which is of course not desirable in a practical application, where parameters can be controlled with limited accuracy only. The nonexistence of a solution usually causes the "checker-board problem" in topology design (cf. [9]), i.e., the solution changes with the grid and develops a checker-board type structure for fine grids (cf. [10] for a general discussion, and [11] for a specific example related to waveguides).

In order to compensate the ill-posedness of the problem, regularization methods have to be used to compute a stable approximation of the solution (or to obtain the existence of a solution at). The main idea of regularization is to solve a well-posed problems that is close to the original one. For a detailed discussion of ill-posedness and regularization we refer to [12]. A frequently used approached is Tikhonov-regularization (or penalization), which consists in minimizing

$$J_{\alpha}(\Lambda, U; q) := J(\Lambda, U; q) + \alpha R(q) \to \min_{\Lambda, U, q},$$
(3)

where R is a suitable (convex) regularization functional. If q is a distributed variable, the typical choices for R are of the form

$$R(q) = \int_D \left| Lq(x) \right|^2 dx,$$

where *L* is either the identity or a differential operator such as  $L = \nabla$ . If piecewise constant design variables *q* are desired, one can use the total variation penalty (cf. [13])

$$R(q) = \int_D |\nabla q(x)| \, dx,$$

or directly model the design variable as a piecewise constant function and add the perimeter of its discontinuities (i.e., the length of the curve in 2D and surface area in 3D) as a penalty. Note that the bounded variation penalty is equal to jump height times times length of the discontinuity curve for piecewise constant design variables, and therefore essentially equivalent to penalization by perimeter. The different possibilities of modelling the design variable are discussed in the following section.

# 2.2 Models of the Design Variable

In many optimal design problems the natural design variable is the distribution or mixture of materials, which is also the case for photonic crystals. The natural model for the design variable in such cases is a piecewise constant function q, with well-defined values in each phase defined by the specific materials. The free variable that can be optimized is then the geometry of the phases, which can be carried out in several different ways. For simplicity we restrict our attention to the case of two phases in the following, but similar reasoning is possible for multiple phases, too. In this case, we can split the domain D into  $\overline{D} = \overline{\Omega_1} \cup \overline{\Omega_2}$ , with open sets  $\Omega_j$  representing the different materials. The function qis defined by

$$q(x) = \begin{cases} q_1 & x \in \Omega_1 \\ q_2. & x \in \Omega_2. \end{cases}$$
(4)

The design problem reduces to the problem of distributing the phase  $\Omega_1$  in D (the second phase is clearly the complement of  $\Omega_1$ ), which is usually denoted by the terms shape or topology optimization (cf. [10], [14]). The approach in classical shape optimization usually starts from a fixed topology and tries to find a local minimizer by (local) variations of the boundary  $\partial\Omega$ . In general topology optimization, the shape of the boundary of the phases is optimized as well as their topological structure such as the number of connected components. As a representation of the design variable  $\Omega_1$ , the following methods can be used:

- Parameterization: A simple method consists in choosing an a-priori parameterization of the boundary ∂Ω<sub>1</sub> and optimization of the parameters. This yields a rather standard optimization problem of lower dimension, but strongly restricts the topology of the phase. In particular in applications to photonic crystals, where the number of crystals is not specified a-priori, this is not a desirable property. Nonetheless, this approach has been used for the optimization of photonic crystals (cf. [15]–[17]) with additional mechanisms to change topologies, which creates computational complications. On the other hand, parameterization has proved to be useful in the shape optimization of waveguides when the shape shall be changed only locally (cf. [11]).
- *Level Set Methods:* The main idea of the level set approach (cf. [18], [19]) is to represent the phase as the zero level set of a continuous function φ, i.e.,

$$\Omega_1 = \{ x \in D \mid \phi(x) < 0 \}.$$
(5)

By allowing additional time-dependence of  $\phi$ , one can compute geometric motion of  $\Omega_1$  in time by evolving the level set set function  $\phi$ . A geometric motion with normal velocity V = V(x, t) can be realized by solving the Hamilton-Jacobi equation

$$\frac{\partial \phi}{\partial t} + V |\nabla \phi| = 0. \tag{6}$$

Optimization within the level set framework consists in choosing a velocity V driving the evolution towards a minimum (or at least decreasing the objective). There are various possibilities to choose the velocity in order to obtain a descent, we refer to [20], [21] for a detailed discussion.

• Approximation of the Indicator Function: Several methods have been devised to directly approximate the indicator function  $\chi$  of  $\Omega_1$ , respectively the piecewise continuous function  $q = q_1\chi + q_2(1 - \chi)$ . A frequently used method in structural optimization is the SIMP approach (Solid Isotropic Material with Penalization), which optimizes a spatially dependent density  $\tilde{\rho}(x)$  such that  $\rho(x) = r\tilde{h}o(x)^p$ , with p > 1. This power law for the density forces densities close to 0 - 1 distributions. In structural optimization, it has been shown by Bendsoe and Sigmund [22], that this power law approach is physically permissible as long as some conditions on the power in dependence of the Poisson ration of the material are satisfied, a similar analysis for photonic applications is not available yet.

Another possibility of approximating the indicator function is the phase-field approach used by Bourdin and Chambolle [23] for structural optimization. In this case, an additional term is added to the objective functional, penalizing deviations of  $\rho(x)$  from the values  $\rho_1$  and  $\rho_2$ .

If fine mixtures of phases are allowed, one can choose a different approach and allow for a general spatially dependent density q = q(x) satisfying

$$\min\{q_1, q_2\} \le q(x) \le \max\{q_1, q_2\}.$$
(7)

This density q can be interpreted as a limit of fine mixtures in the sense of homogenization. The numerical solution is rather straightforward in this case, since the function qcan be discretized directly as well as the state, which finally yields a standard nonlinear programming problem with the additional bound constraints for the discretization of q. On the other hand, the homogenization approach suffers from several drawbacks. In particular, it can be made rigorous only for a limited class of objective functionals and gives no control on the fineness of details. We refer to the monograph of Allaire [24] for a detailed discussion of the homogenization method.

# 2.3 Optimization Techniques

After modelling the design variable and the regularization

term, one ends up with a nonlinear optimization problem, which is well-posed due to the regularization term, but probably ill-conditioned for small values of the regularization parameter. In principle, any suitable optimization method can be chosen to solve these optimization problems, but the optimal choice should of course depend on the regularization term and the model of the design variable. E.g., if a total variation penalty term is used, the regularization term involves a nondifferentiability and hence, a method using higher order derivatives is not appropriate. On the other hand, models of the design variable such as the phasefield model may introduce strong non-convex terms into the model, so that standard Newton-type methods may run into difficulties.

Another difference between design variables dependent on a shape and intermediate densities is the appearance of constraints. If the design variable is modeled as a piecewise constant function such as in the level set method, the only constraint that might remain is a bound on the volume, which can be incorporated easily. If intermediate densities are used, the inequality constraints (7) have to be incorporated. Therefore, sequential linear or convex programming methods like CONLIN (cf. [25]) or MMA (cf. [26], [27]) are more popular in these cases than Newton-type or other sequential quadratic programming methods.

Nonetheless, there are some common properties of all approaches, which we shall discuss in the following. The standard approach consists in (implicitly) eliminating the state variable U and the eigenvalues  $\Lambda$ , which are uniquely determined for a given design q. Therefore, with the notation U(q) and  $\Lambda(q)$  for the unique solution of the eigenvalue problem with given q, one can reformulate the design problem purely in terms in q as

$$\tilde{J}_{\alpha}(q) := J(\Lambda(q), U(q); q) + \alpha R(q) \to \min_{\alpha} .$$
(8)

In order to compute derivatives of the functional  $\tilde{J}_{\alpha}$  one has to compute the derivatives of U and A with respect to q, since

$$\begin{split} \tilde{J}'_{\alpha}(q)h &= \frac{\partial}{\partial q} J(\Lambda(q), U(q); q)h \\ &+ \frac{\partial}{\partial U} J(\Lambda(q), U(q); q)U'(q)h \\ &+ \frac{\partial}{\partial \Lambda} J(\Lambda(q), U(q); q)\Lambda'(q)h + \alpha R'(q)h. \end{split}$$

Here U'(q)h and  $\Lambda'(q)h$  denote the derivatives of the state and eigenvalues with respect to the design variable q in direction h. These derivatives can be computed from a linearization of the state Eq. (2), for simplicity we omit the dependence on q and h in the notation:

$$\begin{aligned} A(u'_{j};q) &= -\frac{\partial}{\partial q} A(u_{j};q)h + \lambda'_{j} B(u_{j};q) \\ &+ \lambda_{j} B(u'_{j};q) + \lambda_{j} \frac{\partial}{\partial q} B(u_{j};q)h \end{aligned}$$

Here we simply denote the directional derivatives by

 $u'_j$  and  $\lambda'_j$ . Thus, one obtains a similar linear problem to be solved for the derivatives U'(q)h and  $\Lambda'(q)h$ , for each variation *h*. Solving all these linear problems for all possible variations would cause an unreasonable computational effort, but fortunately this problem can be avoided by using the so-called adjoint method. First of all, one can use the symmetry of the operators *A* and *B* to deduce that

$$\langle A(u'_j;q) - \lambda_j B(u'_j;q), u_j \rangle = \langle A(u_j;q) - \lambda_j B(u_j;q), u'_j \rangle = 0.$$

where  $\langle .,. \rangle$  denotes the  $L^2$ -inner product. Hence, we can eliminate the terms depending on U' from the linearized equation to obtain

$$\lambda'_{j}\langle B(u_{j};q),u_{j}\rangle = \left\langle -\frac{\partial}{\partial q}A(u_{j};q)h,u_{j}\right\rangle$$
$$+\lambda_{j}\left\langle \frac{\partial}{\partial q}B(u_{j};q)h,u_{j}\right\rangle$$

1 0

This relation can be used to compute the derivatives of the eigenvalues with respect to the design - note that it only depends on the known values q, U(q), and  $\Lambda(q)$ .

# 3. Optimal Design of Photonic Crystals

In general, a photonic crystal can be viewed as a low-loss dielectric medium with several air inclusions, which are the principle design variables. There are several design goals related to photonic crystals, leading to inverse wave problems or inverse spectral problems (cf. [28]). In the following we shall discuss the two main classes, namely the optimization of bandgap structures and the optimization of waveguide structures. We shall review the (few) existing papers using inverse problems techniques for these problems. Finally, we discuss some model problems related to the Helmholtz equation, which allow further insight into basic problem structure.

The standard model for the electromagnetic waves in photonic crystals are the Maxwell-Equations, which can under standard constitutive relations and for the assumption of monochromatic waves be reduced to the following stationary system for the electric and magnetic fields **E** and **H**:

$$\begin{pmatrix} \frac{\omega}{c} & \frac{i}{\epsilon} \nabla^{\times} \\ -\frac{i}{\mu} \nabla^{\times} & \frac{\omega}{c} \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = 0,$$
(9)

on the space of divergence-free vector fields **E** and **H**. Here,  $\nabla^{\times}$  denotes the curl operator, *c* is the speed of light,  $\omega$  the frequency of the wave,  $\epsilon$  and  $\mu$  are the electric and magnetic permittivity of the photonic crystals. The latter parameters can be modeled as scalar function of the location, whose value is determined by the current phase (i.e., material or air-inclusions). For most photonic crystal it is assumed that the material is nonmagnetic, i.e.,  $\mu \equiv 1$ . Thus, the design variable enters the model mainly via the electric permittivity, which can be modeled as a piecewise constant function taking different (fixed) values in the material and the air inclusions. For two-dimensional structures, there are two-possible reductions. In the case of transverse electric (TE) polarized fields, the magnetic field is along the  $x_3$  axis and the electric field is normal to this axis. The Maxwell system can then be reduced to a divergence-type problem for the variable  $u = H_3$  of the form

$$-\nabla . \frac{1}{\epsilon} \nabla u = \lambda u, \tag{10}$$

in two dimensions, with  $\lambda = \omega/c$ . For transverse magnetic (TM) polarized fields, the electric field is parallel and the magnetic field normal to the  $x_3$ -axis. In this case, ther three-dimensional Maxwell equations reduce to the two-dimensional problem

$$-\Delta u = \lambda \epsilon u, \tag{11}$$

for the scalar function  $u = E_3$ .

### 3.1 Optimal Design of Bandgap Structures

A photonic bandgap structure (PBG) is a periodic photonic crystal, in which electromagnetic waves of certain frequencies cannot propagate. In order to deal with the periodic media, so-called Bloch waves are used (cf. [29], [30] for details), which allow to solve equations on the unit square instead. The basic idea of this theory is that solutions on the whole space are superpositions of the solutions ( $\mathbf{E}_{\alpha}, \mathbf{H}_{\alpha}$ ) on the unit cell of

$$\frac{\iota}{\epsilon} (\nabla + i\alpha) \times \mathbf{H}_{\alpha} = \lambda \mathbf{E}_{\alpha}, (\nabla + i\alpha) \cdot \mathbf{H}_{\alpha} = 0$$
(12)

$$-\frac{i}{\epsilon}(\nabla + i\alpha) \times \mathbf{E}_{\alpha} = \lambda \mathbf{H}_{\alpha}, (\nabla + i\alpha).\mathbf{E}_{\alpha} = 0,$$
(13)

for all  $\alpha \in K = [-\pi, \pi]^3$  (*K* is usually called Brillouin zone), with the eigenvalue  $\lambda = \omega/c$ . Thus, bandgap materials can be computed on the unit cell at the price of having to compute the solution for all  $\alpha \in K$ .

A typical design goal is to obtain a maximal bandgap around a given frequency  $\omega_0$ . In spatial dimension two, Cox and Dobson [31], [32] used the objective functional

$$J(\Lambda(q)) = \inf_{\alpha \in K_0} \min\{\omega_0 - \lambda_{k-1}(q, \alpha), \lambda_k(q, \alpha) - \omega_0\},\$$

where  $K_0$  is a suitable subset of the first Brillouin zone  $[-\pi, \pi]^2$ . An analysis of the problem shows that the problem may be non-smooth, i.e., Lipschitz-continuous but not differentiable with respect to the design variable, for several reasons. First of all, the infimum and minimum in the above formula for *J* are non-smooth functions. Moreover, multiple eigenvalues introduce a non-differentiability with respect to the design variable as we have seen above. However, one can still use generalized gradients and bundle optimization techniques to overcome this difficulty (cf. [33]). The model of the design variable in [31], [32] was a continuous density variable constrained by (7), i.e. the electric permittivity in the case of TM-polarization (investigated in [31]) and its reciprocal value in the case of TE-polarization (investigated

in [32]). The numerical results in both cases are promising, and the obtained densities are close to piecewise continuous functions, i.e., permittivities that can actually be realized. The results demonstrate that inverse problems techniques can be employed to design optimal bandgap structures in an automatic way. Nonetheless, a variety of open problems remains to be investigated for the optimal design of photonic crystals, in particular the three-dimensional case, which is a truly large-scale problem, is of high importance for applications. This poses a strong demand on the efficiency of the eigenvalue solvers as well as of the optimization techniques.

Doosje et al. [15] considered crystals with cubic lattices of air inclusions of radius R, connected by cylindrical pieces of radius  $R_C$ . Their model of the design variable is therefore a simple parametrization, with the radii R and  $R_C$ , as well as the distance *a* between the centers of the balls to be minimized. For the maximization of the gap between the bands 8 and 9, they obtained a maximum occurs for aratios  $R_c/R = 0.398$  and R/a = 0.32, significantly improving their initial design to a relative bandgap of 9.59% around the central frequency  $\omega_0 = 2\pi \times 0.746 c/a$ . Since, the optimization is restricted to 3 parameters in this case, the bandgaps could be increased allowing for more general shapes. E.g., it seems promising to use the results of [15] as a starting point for a shape optimization by the level set method. To our knowledge, the results in [15] represent the only existing work on optimal design of photonic crystals in 3D.

A related problem in mechanics has been investigated by Sigmund and Jensen [34] in phononics, where a similar analysis performed for the elasticity system. So far, phononic structures do not have existing technological applications, but a promising potential of such. From a mathematical viewpoint, the optimal design problem is analogous to the one for photonic crystals and therefore, developments in both areas might influence each other in the future.

Finally, a problem of future interest may be the optimal design of localized defect modes (cf. [35], [36]), which has not yet been discussed in full generality but only for a simple model problem that will be discussed in Sect. 3.3.

#### 3.2 Optimal Design of Waveguides

In typical applications to waveguides, one does not seek periodic structures, but rather finite structures. The design goal in this case is the guidance of a mode through the device with minimum power loss (cf. [11], [16]), in many cases of the first fundamental mode. Since the structure is usually not assumed to be periodic in this case, the model does not involve Bloch waves and consists simply of the Maxwell equations on a domain  $\Omega$  modelling the device geometry.

There are two possible design variables for waveguide devices: the topology of the photonic crystal (i.e., the air inclusions) and the overall device geometry  $\Omega$ . While the first problem is a typical topology design problem as described above, the design of the device geometry is rather a classical shape optimization problem, where no change of the topological structure is desired. Therefore it seems reasonable

to use parametrizations and to optimize locally around the initial shape. This approach was used with success by Felici and Engl [11] together with an appropriate regularization of the parameters to avoid the checker-board problem described above.

The design of photonic crystals in waveguide structures has been investigated recently by Felici and Gallagher [16]. The authors used the radii and the locations of some of the air inclusions as design variable, while most of the air inclusions were fixed on a hexagonal lattice. The authors used fast local optimization techniques together with stochastic and deterministic global optimization techniques to compute global minima in reasonable times.

#### 3.3 Model Problems for the Helmholtz Equation

Several inverse problems related to the Helmholtz equation on a bounded domain have been investigated recently. A simple model for the design of bandgap structures is the maximization of eigenvalues considered by Osher and Santosa [37]. The authors discussed the case of a Helmholtz equation in a bounded domain  $\Omega$ , i.e.,

$$\Delta u = \lambda q u, \tag{14}$$

subject to homogeneous Dirichlet boundary condition. In this case the design variable q was modelled explicitly as a piecewise constant function satisfying (4), and the level set method was used to represent the shapes  $\Omega_j$ . Thus, the density q can be written as

$$q = q_1 + (q_2 - q_1)H(\phi),$$

where H denotes the Heaviside function. The maximization of a band gap corresponds roughly speaking to the minimization of the functional

$$J(\Lambda) = \lambda_k - \lambda_{k-1} \tag{15}$$

subject to a volume constraint. As an alternative way of improving bandgap materials, the author considered the minimization of the volume fraction of one material subject to a fixed size of the "bandgap," i.e., of the difference  $\lambda_k - \lambda_{k-1}$ . The latter design goal models the aim of obtaining a given bandgap as cheap as possible.

The computation of derivatives is particularly simple in this case, since one only needs the derivatives of the eigenvalues  $\lambda_i$ , which satisfies

$$a_j = \frac{\int_{\Omega} |\nabla u_j|^2 \, dx}{\int_{\Omega} q \, u_j^2 \, dx}.$$

By similar reasoning as in Sect. 2 one obtains that

$$\lambda'_{j} = -\int_{\Omega} q' \ u_{j}^{2} \ dx \frac{\int_{\Omega} |\nabla u_{j}|^{2} \ dx}{\int_{\Omega} q \ u_{j}^{2} \ dx} = -\lambda_{j} \int_{\Omega} q' \ u_{j}^{2} \ dx,$$

where q' is the derivative of q with respect to a variation of  $\phi$ . Thus, one can compute the derivative of the objective

functional  $J(\Lambda)$  without solving any additional differential equation. This formula for the derivatives of the eigenvalues were the basis for the level set algorithm applied to this shape optimization problem in [37]. According to the standard level set framework, an evolution of the form

$$\frac{\partial \phi}{\partial t} + V |\nabla \phi| = 0$$

was used with a speed function V of the form

$$V = (q_1 - q_2)(\lambda_k u_k^2 - \lambda_{k-1} u_{k-1}^2) + \eta,$$

with a Lagrange parameter  $\eta$  guaranteeing volume conservation in the evolution. This evolution turned out be successfull in finding optimal shapes, even without a-priori knowledge of the topology. The obtained results by this technique can be realized immediately, since the solution is a decomposition of the geometry into the two materials. Many of the optimal structures obtained by this inverse problems approach are to some extent non-intuitive and difficult to be guessed by engineers, which demonstrates again the importance of automatic inverse problems techniques for design problems of this type. For two cases, namely the maximization of the bandgap between the first two eigenvalues and the minimization of the volume at fixed bandgap are shown in Figs. 1 and 2, respectively. One observes that the optimal structure (last figure at the bottom) has a completely different topology as the starting value (first figure at the top).

Another problem of interest is the optimal design of localized defect modes. A model problem related to the Helmholtz equation has been investigated recently by Dobson and Santosa [38]. In order to measure the locality of the defect mode, the functional

$$J(u,q) = \int_{\Omega} w \, q \, u^2 \, dx$$

was introduced, where u is a solution of the eigenvalue problem (14) and w is an appropriate weight-function such as  $w(x) = |x - x_0|$  with  $x_0$  being the point around which the mode is to be localized. The analysis in [38] shows that this optimal design problem is ill-posed, since there may exist eigenfunctions corresponding to higher and higher frequencies and associated densities q that drive the functional J to zero, but do not converge to any optimal design. In order to regularize the problems, constraints on the eigenvalue have to be enforced, two possible regularization approaches are presented in [38] leading to successful optimal designs. For more realistic situations in photonic crystals one has to expect the same kind of problem, so that these initial results on the Helmholtz equation may help in the construction of optimal designs for practical applications, too.



**Fig.1** Maximization of  $\lambda_2 - \lambda_1$  for the Helmholtz equation. The figure show the evolving partition during the iterations of the level set method (from [37]).



**Fig. 2** Minimization of volume at fixed bandgap  $\lambda_2 - \lambda_1$  for the Helmholtz equation. The figure show the evolving partition during the iterations of the level set method (from [37]).

#### Acknowledgements

Financial support is acknowledged by ONR MURI grant # N00014-02-1-0720 and NSF grant # DMS0074735.

#### References

- S. John, "Strong localization of photons in certain disordered dielectric superlattices," Phys. Rev. Lett., vol.58, pp.2486–2489, 1987.
- [2] E. Yablonovitch, "Inhibited spontaneous emission in solid-state physics and electronics," Phys. Rev. Lett., vol.58, pp.2059–2062, 1987.
- [3] C.M. Bowden, J.P. Dowling, and H.O. Everitt, eds., "Development and applications of materials exhibiting photonic band gaps," J. Opt. Soc. Am. B, vol.10, no.2, pp.280–413, 1993.
- [4] J.D. Joannopoulos, R.D. Meade, and J.N. Winn, Photonic Crystals: Molding the Flow of Light, Princeton University Press, 1995.
- [5] E. Yablonovitch, "Photonic crystals: Semiconductors of light," Scient. Am., vol.285, pp.34–41, 2001.
- [6] P. Kuchment, "The mathematics of photonic crystals," in Mathematical Modeling in Optical Science, ed. G. Bao, L. Cowsar, and W. Masters, pp.207–272, SIAM, Philadelphia, 2001.
- [7] D.C. Dobson, "An efficient method for band structure calculations in 2D photonic crystals," J. Comp. Phys., vol.149, pp.363–376, 1999.
- [8] D.C. Dobson, J. Gopalakrishnan, and J.E. Pasciak, "An efficient method for band structure calculations in 3D photonic crystals," J. Comp. Phys., vol.161, pp.668–679, 2000.
- [9] O. Sigmund and J. Petersson, "Numerical instabilities in topology optimization: A survey on procedures dealing with checkerboards, mesh-dependencies and local minima," Struct. Optim., vol.16, pp.68–75, 1998.
- [10] M.P. Bendsoe and O. Sigmund, Topology Optimization, Springer, Berlin, Heidelberg, New York, 2003.
- [11] T. Felici and H.W. Engl, "On shape optimization of optical waveguides using inverse problem techniques," Inverse Probl., vol.17, no.4, pp.1141–1162, 2001.
- [12] H.W. Engl, M. Hanke, and A. Neubauer, Regularization of Inverse Problems, Kluwer, Dordrecht, 1996.
- [13] L.I. Rudin, S.J. Osher, and E. Fatemi, "Nonlinear total variation based noise removal algorithms," Physica D, vol.60, pp.259–268, 1992.
- [14] B. Mohammadi and O. Pironneau, Applied Shape Optimization for Fluids, Clarendon Press, Oxford, 2001.
- [15] M. Doosje, B.J. Hoenders, and J. Knoester, "Photonic bandgap optimization in inverted fcc photonic crystals," J. Opt. Soc. Am. B, vol.17, no.4, pp.600–606, 2000.
- [16] T. Felici and T.F.G. Gallagher, "Improved waveguide structures derived from new rapid optimization techniques," Proc. SPIE, vol.4986, 2003, to appear.
- [17] J.M. Geremia, J. Williams, and H. Mabuchi, "Inverse problems approach to designing photonic crystals for cavity QED experiments," Phys. Rev., vol.E66, no.066606, pp.1–12, 2002.
- [18] S.J. Osher and J.A. Sethian, "Fronts propagating with curvaturedependent speed: Algorithms based on Hamilton–Jacobi formulations," J. Comp. Phys., vol.79, pp.12–49, 1988.
- [19] S.J. Osher and R. Fedkiw, The Level Set Method and Dynamic Implicit Surfaces, Springer, New York, 2002.
- [20] F. Santosa, "A level-set approach for inverse problems involving obstacles," ESAIM: Control, Optimisation and Calculus of Variations, vol.1, pp.17–33, 1996.
- [21] M. Burger, "A framework for the construction of level set methods for shape optimization and reconstruction," Interfaces and Free Boundaries, vol.5, no.3, pp.301–329, 2003.
- [22] M.P. Bendsoe and O. Sigmund, "Material interpolations in topology optimization," Arch. Appl. Mech., vol.69, pp.635–654, 1999.

- [23] B. Bourdin and A. Chambolle, "Design-dependent loads in topology optimization," ESAIM: Control, Optimization and Calculus of Variations, vol.9, no.1, pp.19–48, 2003.
- [24] G. Allaire, Shape Optimization by the Homogenization Method, Springer, New York, 2002.
- [25] C. Fleury, "CONLIN: An efficient dual optimizer based on convex approximation concepts," Struct. Optim., vol.1, pp.81–89, 1989.
- [26] K. Svanberg, "The method of moving asymptotes—A new method for structural optimization," Int. J. Numer. Methods Eng., vol.24, pp.359–373, 1987.
- [27] K. Svanberg, "A class of globally convergent optimization methods based on conservative convex separable approximations," SIAM J. Optim., vol.12, no.2, pp.555–573, 2002.
- [28] J. McLaughlin, "Solving inverse problems with spectral data," in Surveys on Solution Methods for Inverse Problems, ed. D. Colton, H. Engl, A.K. Louis, J. McLaughlin, and W.F. Rundell, pp.169–194, Springer, New York, 2000.
- [29] A. Bensoussan, J.L. Lions, and G. Papanicolaou, Asymptotic analysis for periodic structures, North-Holland Publishers, Amsterdam, New York, Oxford, 1978.
- [30] P. Kuchment, Floquet Theory for Partial Differential Equations, Birkhäuser, Basel, 1993.
- [31] S.J. Cox and D. Dobson, "Maximizing band gaps in twodimensional photonic crystals," SIAM J. Appl. Math., vol.59, no.6, pp.2108–2120, 1999.
- [32] S.J. Cox and D.C. Dobson, "Band structure optimization of twodimensional photonic crystals in H-polarization," J. Comp. Phys., vol.158, no.2, pp.214–224, 2000.
- [33] F. Clarke, Optimization and Nonsmooth Analysis, SIAM, Philadelphia, 1990.
- [34] O. Sigmund and J.S. Jensen, "Systematic design of phononic bandgap materials and structures by topology optimization," Philos. Trans. R. Soc. Lond. A, Math. Phys., vol.361, no.1806, pp.1001– 1019, 2003.
- [35] A. Figotin and A. Klein, "Localized classical waves created by defects," J. Stat. Phys., vol.86, pp.165–177, 1997.
- [36] A. Figotin and A. Klein, "Midgap defect modes in dielectric and acoustic media," SIAM J. Appl. Math., vol.58, pp.1748–1773.
- [37] S.J. Osher and F. Santosa, "Level set methods for optimization problems involving geometry and constraints. I. Frequencies of a twodensity inhomogeneous drum," J. Comput. Phys., vol.171, no.1, pp.272–288, 2001.
- [38] D. Dobson and F. Santosa, "Optimal localization of eigenfunctions in an inhomogeneous medium," Preprint, 2003.



**Martin Burger** received his master and Ph.D. (2000) from Johannes Kepler University Linz, Austria. After working at the Universities of Milano and Linz, and completing his civil service, he is currently assistant professor at UCLA. Dr. Burger has been working on the numerical solution of applied inverse and optimal design problems, as well as on the modeling and simulation of problems in materials science (polymers, semiconductors). He was awarded a price for special student achievements by the

Austrian Ministry of Science in 1999.



Stanley J. Osher received his M.S. and Ph.D. (1966) from the Courant Institute, NYU. After working at Brookhaven National Laboratory, UC Berkeley and SUNY Stony Brook, he has been at UCLA since 1976. He is Director of Special Projects at the Institute for Pure and Applied Mathematics at UCLA. Dr. Osher is the coinventor of i) level set methods for computing moving fronts (8600 references on GOOGLE, ii) ENO, WENO and other numerical methods for computing solutions to hyperbolic conserva-

tion laws and Hamilton-Jacobi equations, iii) total variation and other PDE based image processing techniques. He has been a Fulbright and Alfred P. Sloan Fellow, received the NASA Public Service Group Achievement Award, Japan Society of Mechanical Engineers Computational Mechanics Award, was an invited speaker at the International Congress of Mathematicians and recently received the SIAM Pioneer Prize at the ICIAM conference last summer. He has cofounded 3 companies, based, in part, on his own research. His work has been written up numerous times in the scientific and international media, e.g., Science News, Die Zeit (1999). He is a highly cited researcher according to web-of-science.



**Eli Yablonovitch** is Professor of Electrical Engineering at the UCLA Electrical Engineering Dept. Previously he was he was a Distinguished Member of Staff, and also Director of Solid-State Physics at Bell Communications Research. He was also Assoc. Prof. of Applied Physics at Harvard, and held other research & management positions in American industry. Among his honors are an Alfred P. Sloan fellowship (1978–1979), the Adolf Lomb Medal of the Optical Society of America (1978), an

R&D 100 award (1990), the W. Streifer Scientific Achievement award of the IEEE/LEOS (1993), and the R.W. Wood Prize of the Optical Society of America (1996), the Clifford Paterson Lecturer of the Royal Society of London (2000), and the Julius Springer Prize in Applied Physics (2001). He has been named a Fellow of the Institute of Electrical and Electronic Engineers (1992), the American Physical Society (1990), and the Optical Society of America (1982). He is a member of the National Academy of Engineering (2003), the National Academy of Sciences (2003), and is a Life Member of Eta Kappa Nu. Eli Yablonovitch has covered a broad variety of research topics: nonlinear optics, laser-plasma interaction, infrared laser chemistry, photovoltaic energy conversion, strained-quantum-well lasers, and chemical modification of semiconductor surfaces. Currently his main interests are in optoelectronics, high speed optical communications including optical code division multiplexing, photonic crystals, nano-photonics in general including advanced optical lithography, quantum computing and quantum communication, and spin-based electronics.