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Optimal Design of Photonic Band-Gap Structure Based on Kriging Surrogate Model

Hongxia Li[1], Bao Zhu[2], and Jiefu Chen[3, *]

Abstract—Toward an engineering optimization for photonic band-gap structures in waveguide filter, this paper presents an effective optimization method using Kriging surrogate model combing with semi-analytical spectral element method to maximize photonic band-gaps. Photonic crystals are assumed to be finite periodic structures composed of two dielectric materials with different permittivities. Kriging surrogate model is used to build an approximate function relationship between the photonic band-gaps and the design parameters of photonic crystals, replacing the expensive reanalysis for electromagnetic simulations of 3D periodic structure. The semi-analytical spectral element method is used to calculate the photonic band-gaps at different sampling points. Numerical results demonstrate that the proposed optimization method can effectively obtain maximum photonic band-gaps.

1. INTRODUCTION

Photonic crystals are periodic optical structures in one, two or three dimensions. Photonic crystals are also named photonic band-gap (PBG) structures because of their ability of allowing or forbidding the propagation of light within certain frequency ranges [1, 2]. The photonic band-gaps in a photonic crystal structure play a vital role to realize various applications [3–5] in the field of optical technology. Specific band-gap is required in practice, so it is of great significance to design photonic band-gaps within certain frequency ranges. The photonic band-gaps depend not only on the properties of dielectric materials in photonic crystals but also the sizes and material distributions [6]. Therefore, in order to obtain large band-gaps in phononic crystals, a structural optimization question is required to be solved: how to find specific refractive indexes of dielectric materials as well as structural parameters to maximize the specific photonic band gap.

The conventional method for design of photonic band gap (PBG) structures is a trial-and-error process based on physical intuitions and parametric studies. This process would be inefficient and specialized [7]. The design based on this process may not be an optimal solution. For infinite periodic photonic crystals, Meng developed a systematic optimal design method based on sensitivity analysis of a periodic unit cell [8]. However, for finite periodic photonic crystals, the entire PBG structure is required to be analyzed rather than only one unit cell, and it can become much more computationally expensive for 3D electromagnetic simulation. Therefore, it is still a challenge to optimize finite periodic PBG structures with any band gap.

In order to optimize the PBG structure efficiently, we use Kriging surrogate models [9] combined with semi-analytical spectral element method (SEM) [10] to construct global approximations for PBG structure optimization. The highly efficient semi-analytical SEM is used to analyze the 3D structures of PBG to obtain the photonic band-gaps at different sampling points, and it can achieve spectral accuracy

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* Corresponding author: Jiefu Chen (chenjiefu@gmail.com).

[1] School of Mechanical Engineering, Dalian University of Technology, Dalian, Liaoning 116023, China. [2] Surface Engineering Laboratory, School of Materials Science and Engineering, Dalian University of Technology, Dalian, Liaoning 116023, China. [3] Department of Electrical and Computer Engineering, University of Houston, Houston, Texas 77004, USA.

with the increase of interpolation order of spectral elements. Kriging surrogate model, a semi-parametric approach that does not rely on any specific model structure, is used to build an approximate function relationship between the photonic band-gaps and the design parameters of photonic crystals, replacing the expensive reanalysis for electromagnetic simulations of 3D periodic structure. The numerical examples are given to demonstrate the efficiency of the proposed optimization algorithm for the design of photonic crystals.

2. METHOD

2.1. Semi-Analytical SEM Analysis

A PBG structure with nine period shown in Fig. 1 is by 0.33 µm rectangular. Each layer of the PBG structure is composed of a dielectric material layer and an air layer. The thicknesses of the air layer and the dielectric material layer along the longitudinal direction are assumed to be a and b, respectively. The circumferential boundary conditions of the PBG structure are PEC. Both ends of the PBG structure are absorbing boundary conditions. The entire PBG structure was decomposed into several layers along the longitudinal direction. Only one 2D 3rd order spectral elements were employed to discretize the cross section for each substructure. The spectral element can avoid the well-known Runge phenomenon and achieve spectral accuracy, which means the numerical results can converge exponentially as the increase of interpolation order of basis functions. A Riccati equation based high precision integration (HPI) method [11] was utilized to perform integration along the longitudinal direction for each substructure, which was the undiscretized direction, to generate the stiffness matrix of the whole PBG structure. No matter how long a substructure is, HPI method for the semi-discretized system can achieve machine precision, i.e., the numerical errors of longitudinal integration by HPI can be as small as the round-off error on a computer. Export stiffness matrices of substructures can be directly assembled to a global system matrix taking the form of block tri-diagonal matrix. A block Thomas algorithm [12] is employed here to solve the final system of equations with very high efficiency to obtain the transmission of the PBG structures.

2.2. Optimization Problem

The aim for designing a photonic crystal is to maximize the band gap at the desired frequency band. Therefore, optimal control model can be formulated as

$$\begin{aligned}
&\text{Minimize } \mathrm{A}_{sb} = \frac{\int_{f_2}^{f_3} S_{21} df}{\int_{f_2}^{f_3} df} \\
&S.t.\ a_1 \le a \le a_2 \\
&b_1 \le b \le b_2 \\
&\varepsilon_r^1 \le \varepsilon_r \le \varepsilon_r^2 \\
&\mathrm{A}_L = \frac{\int_{f_1}^{f_2} S_{21} df}{\int_{f_1}^{f_2} df} \ge T_L \\
&\mathrm{A}_R = \frac{\int_{f_3}^{f_4} S_{21} df}{\int_{f_3}^{f_4} df} \ge T_R
\end{aligned} \tag{1}$$

where a, b, and ε_r are variables of design, where $0 < a \le 1\,\mu\text{m}$, $0 < b \le 1\,\mu\text{m}$ and $0 < \varepsilon_r \le 10$. S_{21} is the transmission coefficient of the PBG structure. f_2 and f_3 are the minimum and maximum frequency of the desired frequency band, where $f_2 = 500\,\text{THz}$ and $f_3 = 700\,\text{THz}$. f_1 and f_4 are the minimum and maximum working frequency of the incident wave, where $f_1 = 300\,\text{THz}$ and $f_4 = 900\,\text{THz}$. A_L and A_R are the mean of transmission coefficient over corresponding frequencies. T_L and T_R are the design allowed minimum mean of transmission coefficient over corresponding frequencies where $T_L = 5\,\text{dB}$ and $T_R = 5\,\text{dB}$.

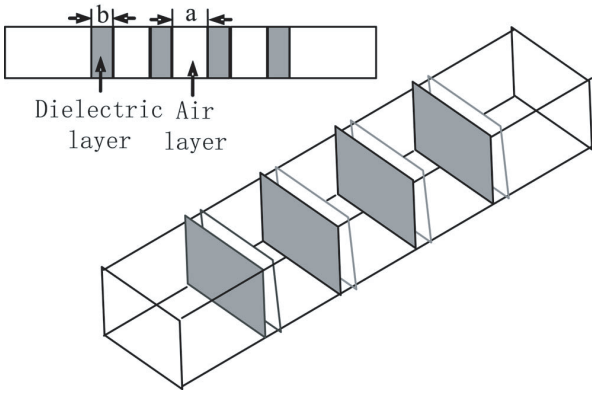

Figure 1. A schematic view of PBG structure.

2.3. Kriging Surrogate Model

The Kriging surrogate model is described as a way of modeling a function as a realization of a stochastic process:

$$\hat{y}(\mathbf{x}^i) = \mathrm{F}(\beta, \mathbf{x}^i) + \mathrm{z}(\mathbf{x}^i) = \mathrm{f}^{\mathrm{T}}(\mathbf{x}^i)\beta + \mathrm{z}(\mathbf{x}^i) \tag{2}$$

where $\mathbf{x}^i = \left\{x_1^i, x_2^i, \ldots, x_m^i\right\}$ is the i-th sample point with variables; $\hat{y}(\mathbf{x}^i)$ is an approximate function fitted to n sample points; $\mathrm{f}^{\mathrm{T}}(\mathbf{x}^i)$ is a linear or nonlinear function of $\mathbf{x}^i$, the superscript T denotes the transpose operator; β is the regression coefficient to be estimated; and $\mathrm{z}(\mathbf{x}^i)$ is the stochastic function, with a mean of zero and a variance σ^2. The spatial correlation function between stochastic functions is given by

$$\mathrm{corr}\left[\mathrm{z}(\mathbf{x}^i), \mathrm{z}(\mathbf{x}^j)\right] = \mathrm{R}(\theta, \mathbf{x}^i, \mathbf{x}^j) = \prod_{l=1}^{m} \exp\left[-\theta(x_l^i - x_l^j)^2\right] \tag{3}$$

where $\mathrm{R}(\theta, \mathbf{x}^i, \mathbf{x}^j)$ is the Gaussian correlation function with θ, which characterizes the spatial correlation between two samples. Parameters can be estimated by maximizing the likelihood of samples.

$$\begin{aligned} \hat{\sigma}^2 &= \frac{\left(\mathbf{y} - \mathbf{f}^{\mathrm{T}}\hat{\beta}\right)^{\mathrm{T}} \mathrm{R}^{-1}\left(\mathbf{y} - \mathbf{f}^{\mathrm{T}}\hat{\beta}\right)}{n} \\ \hat{\beta} &= \frac{\mathbf{f}^{\mathrm{T}}\mathrm{R}^{-1}\mathbf{y}}{\mathbf{f}^{\mathrm{T}}\mathrm{R}^{-1}\mathbf{f}} \\ \hat{\theta} &= \min\left\{\psi(\theta) \equiv |\mathrm{R}|^{\frac{1}{n_s}}\sigma^2\right\} \end{aligned} \tag{4}$$

where $f = [f_1, f_2, \ldots, f_n]$. The estimates $\hat{\beta}$ and $\hat{\sigma}^2$ can then be obtained from Eq. (4).

The function value $\hat{y}(\mathbf{x}^*)$ at a new point $\mathbf{x}^*$ can be approximately estimated as a linear combination of the response values of sample $\mathbf{Y}$

$$\hat{y}(\mathbf{x}^*) = \mathbf{c}^{\mathrm{T}}\mathbf{Y} \tag{5}$$

The mean squared error (MSE) of this predictor is minimized with unbiased estimation, which gives

$$\hat{y}(\mathbf{x}^*) = \mathbf{f}(\mathbf{x}^*)\hat{\beta} + \mathbf{r}(\mathbf{x}^*)^{\mathrm{T}}\gamma \tag{6}$$

where

$$\begin{aligned} \gamma &= \mathbf{R}^{-1}\left(\mathbf{Y} - \mathbf{F}\hat{\beta}\right) \\ \mathbf{r}(\mathbf{x}^*) &= \left[\mathrm{R}(\theta, \mathbf{x}_1, \mathbf{x}^*), \ldots, \mathrm{R}(\theta, \mathbf{x}_n, \mathbf{x}^*)\right] \end{aligned} \tag{7}$$

Thus we can predict the function value $\hat{y}(\mathbf{x}^*)$ at every new point $\mathbf{x}^*$ by using Eq. (6).

2.4. Expected Improvement

The simplest way for optimization is to find the minimum of the response surface which is interpolated through the Kriging method. This way can easily lead to a local minimum, even if iterations are performed. The expected improvement (EI) function [9] is used to balance local and global search. The EI method computes the extent of improvement expected to achieve if sampling at a given point. Before sampling at some point $\mathbf{x}$, the value of $Y(\mathbf{x})$ is unknown. Thus, $Y(\mathbf{x})$ can be regarded as a random variable normally distributed with a mean $\hat{y}(\mathbf{x})$ and variance σ^2 and given by the kriging predictor. If the current best function value is $Y_{\min}$, then we will achieve an improvement of I if $Y(\mathbf{x}) = Y_{\min} - I$. The likelihood of achieving this improvement is given by the normal density function

$$f^{normal}(\mathbf{x}) = \frac{1}{\sqrt{2\pi}\sigma(\mathbf{x})} \exp\left[-\frac{(Y_{\min} - I - \hat{y}(\mathbf{x}))^2}{2\sigma^2(\mathbf{x})}\right] \tag{8}$$

The expected improvement is simply the expected value of the improvement found by integrating over the following density:

$$\mathrm{E}[I(\mathbf{x})] = \int_{I=0}^{I=\infty} I\left\{\frac{1}{\sqrt{2\pi}\sigma(\mathbf{x})} \exp\left[-\frac{(Y_{\min} - I - \hat{y}(\mathbf{x}))^2}{2\sigma^2(\mathbf{x})}\right]\right\} \tag{9}$$

Using integration by parts, one can show that

$$\mathrm{E}[I(\mathbf{x})] = \sigma(\mathbf{x})[u\Phi(u) + \phi(u)] \tag{10}$$

where

$$u = \frac{Y_{\min} - \hat{y}(\mathbf{x})}{\sigma(\mathbf{x})} \tag{11}$$

Φ and ϕ are the normal cumulative distribution and density functions, respectively.

The first term of Eq. (10) is the difference between the current minimum response value $Y_{\min}$ and the prediction $\hat{y}(\mathbf{x})$ at $\mathbf{x}$, penalized by the probability of improvement. Hence, this value is large when $\hat{y}(\mathbf{x})$ is small. The second term is the product of the root mean squared error (RMSE) $\sigma(\mathbf{x})$ and the normal density function $\phi(u)$. The normal density function value is large when $\sigma(\mathbf{x})$ is large and $\hat{y}(\mathbf{x})$ is closed to $Y_{\min}$. Thus, the expected improvement will tend to be large at a point with a predicted value smaller than $Y_{\min}$ and/or when there is a lot of uncertainty associated with the prediction.

2.5. The Convergence Criterion

The convergence criterion is here to satisfy

$$\begin{aligned} &\frac{EI(\mathbf{x}_k)}{Y_{\max} - Y_{\min}} \le \varepsilon_1 \\ &|f(\mathbf{x}_k) - \hat{y}_k| \le \varepsilon_2 \end{aligned} \tag{12}$$

where ε_1 and ε_2 are the convergence tolerances. $Y_{\max}$ and $Y_{\min}$ are the maximal and minimal function values in samples, respectively. $\hat{y}_k$ is the approximate value of the objective function obtained by Kriging model in the k-th iteration. An advantage of this convergence criterion is that the user can set the relative tolerances ε_1 and ε_2 without prior consideration of the magnitudes of the problem response.

2.6. Optimization Algorithm

The optimization algorithm for a PBG structure based on the Kriging model combining with semi-analytical SEM is illustrated in Fig. 2. In this optimization problem, optimal latin hypercube sampling (LHS) method [13] was used to get the sampling points. The semi-analytical SEM simulation can be seen as a black-box, in which design variables are input and the corresponding objective function $\mathrm{A}_{sb}(\mathbf{x})$ is output. Kriging surrogate model was used to construct a global approximate relationship between the objective function $\mathrm{A}_{sb}(\mathbf{x})$ and design variables based on the trial samples. After the approximate relationship was constructed, EI function is used to balance local and global search and tends to find the global optimal design. Sequential quadratic programming optimization algorithm was employed to implement the design optimization based on maximum EI and obtain the modified design variables. The optimization process stops when the convergence criterion is satisfied.

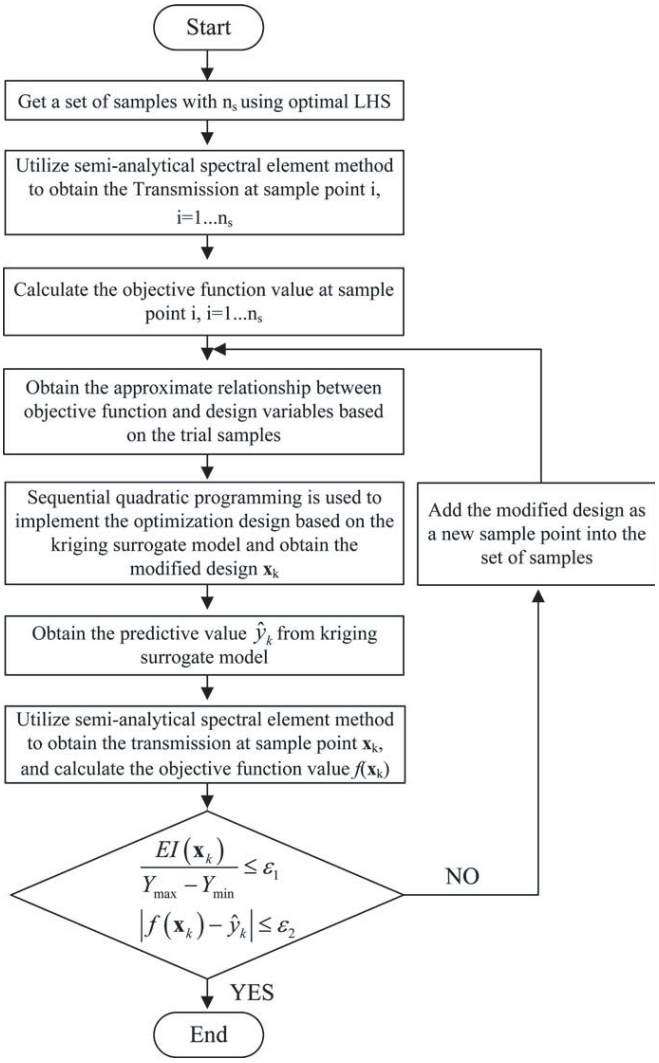

Figure 2. Flow diagram for the optimization method based on Kriging surrogate model combined with semi-analytical spectral element method.

3. RESULTS

The transmission coefficient of the PBG structure in the desired frequency band was minimized by the proposed method shown in Fig. 3. It means that the photonic band-gap is maximized. The initial trial samples shown in Fig. 4 are selected for building Kriging surrogate model, which include a 200 samples selected by the optimal LHS. The transmission coefficient of the PBG structure for all trial samples are obtained by semi-analytical SEM analysis. EI function was employed to balance local and global search for design space. 17 iterations were required to obtain the optimal solution based on optimal LHS as shown in Fig. 5–Fig. 8.

The optimization program stopped when all the criterions described in Fig. 2 were satisfied. The optimization result is shown in Table 1 by comparing to the original design (optimal solution in initial trial samples). The minimum transmission coefficient of the PBG structure in the desired frequency band was reduced from -2.919 dB to -40.265 dB. These results show that this optimization method based on the Kriging surrogate model can effectively reduce the transmission coefficient in the desired frequency band to improve maximize the photonic band-gap of the PBG structure.

Figures 9–11 show the effect of each design variable on the normalized objective function value

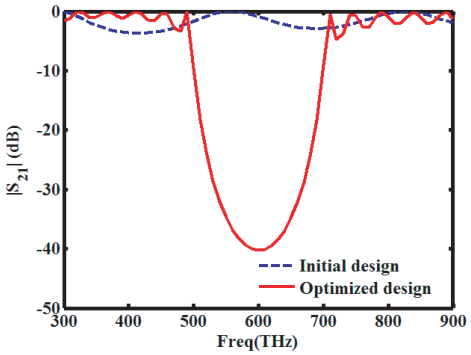

Figure 3. Stop-band characteristic for optimized structure.

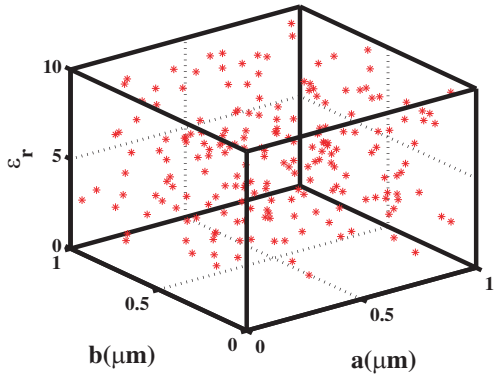

Figure 4. Samples distributions of a optimal LHS approach.

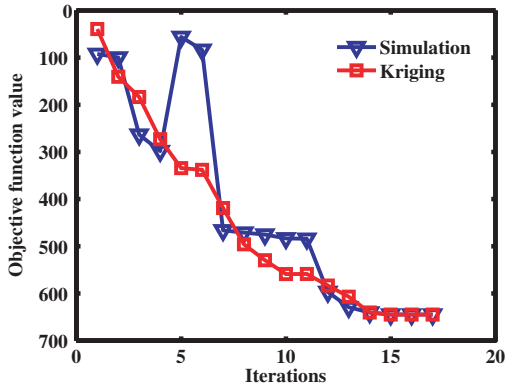

Figure 5. Iterative histories for objective function.

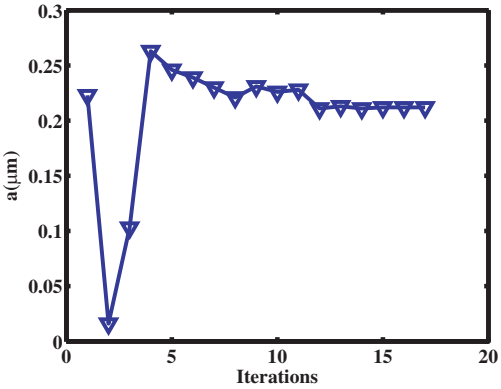

Figure 6. Iterative histories for design variables a.

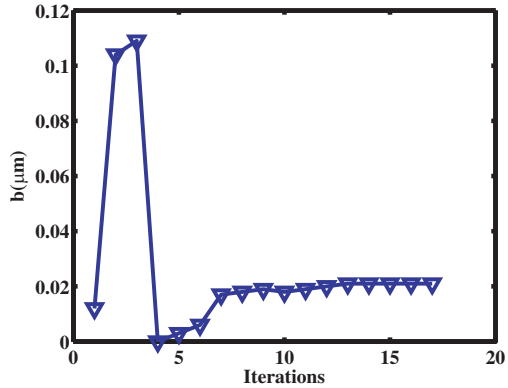

Figure 7. Iterative histories for design variables b

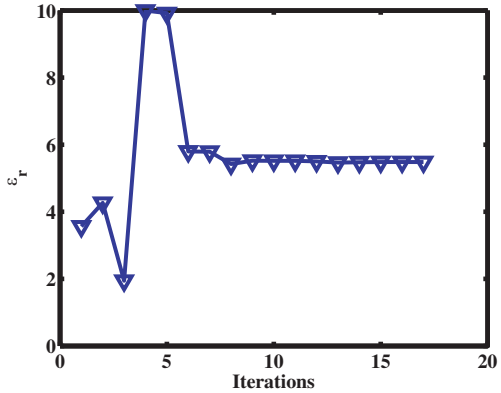

Figure 8. Iterative histories for design variables ε_r.

when fixing other variables at their optimal values. The normalized objective function is defined as

$$A_{sb}^{norm} = \frac{A_{sb} - \min(A_{sb})}{\max(A_{sb}) - \min(A_{sb})} \tag{13}$$

These results show that the objective function value has multiple local optimal solution with the design variable values, because of the complicate nature of the solution space. It is indicated that the optimization method has the ability of global search.

Table 1. Optimization results.

Design variable	a	b	ε_r	Objective function
Initial design	0.070 μm	0.021 μm	6.023	−29.92
Optimized design	0.212 μm	0.021 μm	5.483	−644.8

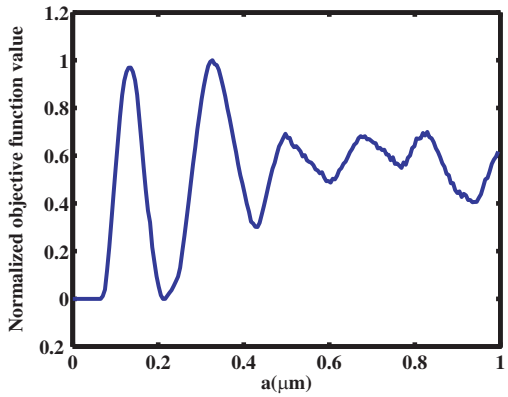

Figure 9. The effect of design variable a on the objective function value when fixing other variables at the optimal values.

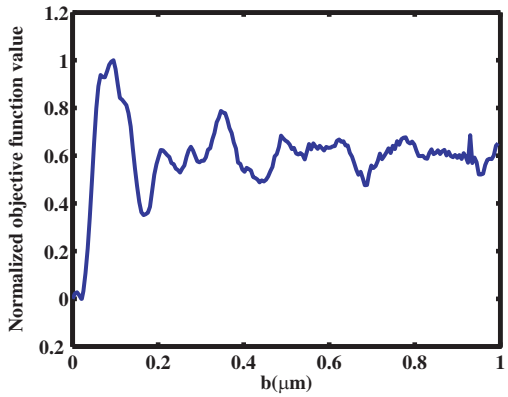

Figure 10. The effect of design variable b on the objective function value when fixing other variables at the optimal values.

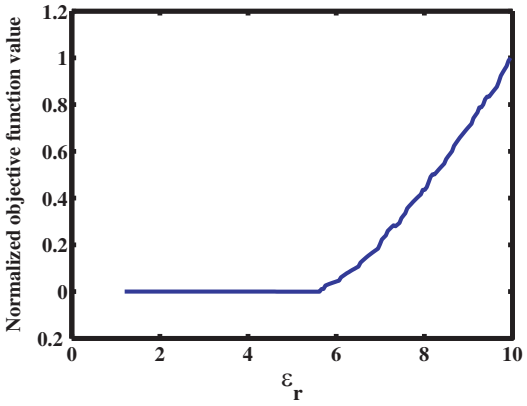

Figure 11. The effect of design variable ε_r on the objective function value when fixing other variables at the optimal values.

4. CONCLUSIONS

This paper investigates the optimization of photonic crystals in waveguide filter. A optimization algorithm based on Kriging surrogate model combing with semi-analytical spectral element method is proposed for the design of PBG structures. Through semi-analytical spectral element analysis, the objective function values of sampling points are efficiently obtained. The optimization algorithm maximized desired band gap of PBG structures without sensitivity analysis. Numerical results indicate that the algorithm proposed in this paper is effective for optimal design of PBG structure in waveguide filter.

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