Photonic crystal device sensitivity analysis with Wannier basis gradients

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We present a powerful sensitivity analysis method for devices in a photonic crystal. The method is based on a Wannier basis field expansion and efficient matrix analysis techniques for finding eigenvalue and transmission gradients with respect to the perturbation. The method permits fast analysis of a large number of dielectric perturbation situations for multiple devices in a photonic crystal. We verify the method with finite-difference time-domain and plane-wave expansion calculations. © 2005 Optical Society of America

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Analysis of performance changes as a result of perturbations, such as fabrication error and temperature-induced index change, is an important step for photonic crystal (PC) structure design. The standard finite-difference approach is to solve directly for the performance parameters before and after perturbations. Often, computationally expensive finite-difference time-domain (FDTD) simulations[1] or plane-wave expansions[2] (PWEs) need to be repeated for each perturbation situation. We show here, however, using a powerful method that we call Wannier basis gradients (WBGs), how multiple perturbation situations can be analyzed at a very small computational cost. This method will permit designers to perform sensitivity analysis on a large variety of perturbations that have often been ignored previously, optimize designs for higher robustness against perturbations and optimize specific performance parameters.

The WBG sensitivity analysis method involves a one-time evaluation of a small perturbation matrix $\mathbf{D}_{\delta 0}{}'$ associated with a particular single unit cell perturbation of a PC. With a few trivial matrix multiplications and shifts involving $\mathbf{D}_{\delta 0}{}'$, we obtain the performance sensitivity to the same perturbation applied to different unit cells or multiple unit cells for any device constructed in the same PC. Furthermore, unlike FDTD simulations and PWE, the WBG method does not require finer computational grids for smaller dielectric boundary perturbations.

Another emerging technique for sensitivity analysis is the finite-difference frequency-domain method,[3] which works well for arbitrary dielectric structures, not just periodic media. The WBG method uses a basis that is optimized for a particular PC. For analyzing multiple designs within a particular PC, it is more efficient to use the WBG method.

For clarity, we focus on defect structures in two-dimensional photonic crystals with TM-polarized fields. Extensions to the TE case[4] and to three dimensions are under investigation. We express the dielectric distribution as $\epsilon(\mathbf{r}) + \sum_i [\Delta \epsilon_i(\mathbf{r})]$, where $\epsilon(\mathbf{r})$ is the dielectric function of the perfect crystal and $\Delta \epsilon_i(\mathbf{r})$ is the defect structure at lattice site i. First we expand the field for the defect mode in maximally localized Wannier basis functions[5] as

$E(\mathbf{r}) = \sum_{n,\mathbf{R}} a_{n,\mathbf{R}} W_{n,\mathbf{R}}(\mathbf{r})$, where $a_{n,\mathbf{R}}$ are the expansion coefficients, and $W_{n,\mathbf{R}}(\mathbf{r})$ are the Wannier functions with Bloch wave band index n and crystal lattice vector $\mathbf{R}$. For resonator structure eigenfrequency calculations, following Busch *et al.*,[6] we solve a sparse (i.e., computationally cheap) eigenvalue equation:

$$\left(\mathbf{I} + \sum_i \mathbf{D}_i \right) \mathbf{a} = \left(\frac{1}{\omega} \right)^2 \mathbf{A} \mathbf{a}, \qquad \mathbf{a} \equiv \{a_{n,\mathbf{R}}\}, \qquad (1)$$

where $\mathbf{I}$ is the identity matrix and ω is the frequency. $\mathbf{A}$ is given explicitly by Busch *et al.*[6] What is important for this discussion is that $\mathbf{A}$ is obtained from the periodic PC properties and it is independent of the defect structure. Matrices $\mathbf{D}_i$ are defined as

$$(\mathbf{D}_i)_{n\mathbf{R},m\mathbf{S}} = \int_{\mathbb{R}^2} W_{n,\mathbf{R}}{}^*(\mathbf{r}) \Delta \epsilon_i(\mathbf{r}) W_{m,\mathbf{S}}(\mathbf{r}) \mathrm{d}^2 \mathbf{r} . \qquad (2)$$

With a few matrix rearrangements, we get a sparse matrix equation for the transmission–reflection of input–output-type devices:

$$\mathbf{B} \mathbf{x} = \mathbf{y} , \qquad (3)$$

where $\mathbf{B}$ is obtained from matrices $\mathbf{A}$ and $\mathbf{D}_i$ and vector $\mathbf{y}$ is a vector related to the input field; $\mathbf{x}$ is a vector of the form $\{\mathbf{r}, \mathbf{t}, \mathbf{a}\}$, where $\mathrm{r} = r_i$, $\mathbf{t} = t_i$, $\{i = 1, 2 \ldots\}$ are reflection and transmission coefficients of the input and output waveguide modes indexed by i. The full form of $\mathbf{B}$ is given by Busch *et al.*[6] What is important for this discussion is that, in the presence of an additional dielectric perturbation $\delta \epsilon(\mathbf{r})$, Eq. (3) becomes

$$(\mathbf{B} + \delta \mathbf{D}) \mathbf{x} = \mathbf{y} , \qquad (4)$$

where $\delta \mathbf{D}$ is given by Eq. (2), with $\delta \epsilon(\mathbf{r})$ in place of $\Delta \epsilon_i(\mathbf{r})$.

The efficiency of the WBG method relies partly on the efficiency of the maximally localized Wannier basis expansion. First, because the Wannier functions are transformations of the Bloch waves, they contain all the information about the underlying crystal. As a

result only a few Wannier basis functions per lattice site are needed to represent the field. Second, because the Wannier functions are highly localized, defects only induce interactions among Wannier functions centered on neighboring lattice sites [Eq. (2)]. This makes the matrices in Eqs. (1) and (3) sparse. The eigenvectors of Eq. (1) and $\mathbf{B}^{-1}$ in Eq. (3) can be calculated with reasonable computational cost, and the results will be used in the WBG sensitivity analysis.

The WBG method can calculate both the sensitivity of the resonator eigenfrequencies and the sensitivity of the transmission–reflection coefficients in input–output-type devices. Consider a single unit cell perturbation $\delta\epsilon_0(\mathbf{r})$ that changes the dielectric distribution to $\epsilon(\mathbf{r}) + \sum_i[\Delta\epsilon_i(\mathbf{r})] + \delta\epsilon_0(\mathbf{r})$. The eigenvalue equation becomes

$$(\mathbf{E} + \mathbf{A}^{-1}\mathbf{D}_{\delta 0})\mathbf{a} = \beta\mathbf{a}, \qquad \beta = (c/\omega)^2, \tag{5}$$

where $\mathbf{E} = \mathbf{A}^{-1}(\mathbf{I} + \sum_i \mathbf{D}_i)$ and $\mathbf{D}_{\delta 0}$ is given by Eq. (2), with $\delta\epsilon_0(\mathbf{r})$ in place of $\Delta\epsilon_i(\mathbf{r})$.

One way to find the sensitivity of the transmission–reflection coefficients is to solve the eigenvalue problem again. However, this method becomes computationally expensive when we apply the same perturbation to other unit cells, or to multiples of them. If we can parameterize the perturbation by parameter γ and find the derivative of $\mathbf{D}_{\delta 0}$ with respect to γ, $\mathbf{D}_{\delta 0}'$, then we can use the WBG method to calculate the effect of the perturbation much more efficiently, without repeating the eigenvalue problem.

One type of easily parameterized perturbation is the scaling of $\Delta\epsilon_n(\mathbf{r})$. This type of perturbation could be caused by effects such as temperature changes or the presence of electric fields. In this case $\mathbf{D}_{\delta 0}' = \mathbf{D}_n$. Another case is a shift in the material boundary. Assuming that γ parameterizes the shift of the material boundary $h(\gamma, \mathbf{r})$, we can show that

$$(\mathbf{D}_{\delta 0}')_{n\mathbf{R}, m\mathbf{S}} = \epsilon_r \oint_{h(\gamma=0, \mathbf{r})} W_{n,\mathbf{R}}{}^*(s)W_{m,\mathbf{S}}(s)\mathrm{d}s, \tag{6}$$

where ϵ_r is the dielectric constant difference across the boundary. This integral is well defined for the TM case, when the electric field is continuous across the material boundary. For TE fields we can use a smoothing method[3,7] to derive a slightly different equation to handle the field discontinuity.

With $\mathbf{D}_{\delta 0}'$ properly defined, let β be a nondegenerate eigenvalue of matrix $\mathbf{E}$ and $\beta(\gamma)$ be an eigenvalue of $\mathbf{E} + \gamma\mathbf{A}^{-1}\mathbf{D}_{\delta 0}'$ such that $\beta(0) = \beta$. β and $\mathbf{E}$ are related by expressions $\mathbf{E}\mathbf{v} = \beta\mathbf{v}$ and $\mathbf{w}^\dagger\mathbf{E} = \mathbf{w}^\dagger\beta$, where $\mathbf{v}$ and $\mathbf{w}$ are the right and left eigenvectors of $\mathbf{E}$ associated with β, respectively. Using a result from matrix analysis,[8] one can show that

$$\frac{\mathrm{d}\beta(\gamma)}{\mathrm{d}\gamma}\bigg|_{\gamma=0} = \frac{\mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{D}_{\delta 0}'\mathbf{v}}{\mathbf{w}^\dagger\mathbf{v}}. \tag{7}$$

Equation (7) is a computationally trivial matrix multiplication, involving $\mathbf{D}_{\delta 0}'$ and a few parameters that are independent of the perturbation and easily

obtained when we calculate the eigenfrequency by use of Eq. (1). Because of the localization of the Wannier functions to a few neighboring unit cells,[6] $\mathbf{D}_{\delta 0}'$ typically has only a few hundred nonzero elements. As a result, the sensitivity analysis can be done in a matter of seconds on modest personal computing hardware.

Although $\mathbf{D}_{\delta 0}'$ is for the perturbation to one specific unit cell, sensitivity analysis of application of the same perturbation to other unit cells, or to multiples of them, is computationally trivial. The change to the dielectric distribution becomes $\sum_j[\delta\epsilon_j(\mathbf{r})]$, where $\delta\epsilon_j(\mathbf{r}) = \delta\epsilon_0(\mathbf{r} - \mathbf{R}_j)$ for the ith unit cell. Using the fact that the Wannier functions for different lattice sites are just translations of each other, we can show that the sensitivity can be evaluated simply as

$$\frac{\mathrm{d}\beta(\gamma)}{\mathrm{d}\gamma}\bigg|_{\gamma=0} = \frac{\mathbf{w}^\dagger\sum_j(\mathbf{A}^{-1}\mathbf{D}_{\delta j}')\mathbf{v}}{\mathbf{w}^\dagger\mathbf{v}}, \tag{8}$$

where $(\mathbf{D}_{\delta j}')_{n\mathbf{R}, m\mathbf{S}} = (\mathbf{D}_{\delta 0}')_{n(\mathbf{R}-\mathbf{R}_j), m(\mathbf{S}-\mathbf{R}_j)}$. The matrix shift is a trivial operation. Therefore we can map the eigenfrequency sensitivity to the perturbation of different unit cells, as well as coherent effects from multiple simultaneous perturbations. Furthermore, the computational overhead of founding $\mathbf{D}_{\delta 0}'$ can be amortized over the analysis of many structures constructed in the same PC.

For small shifts in the material boundary, the direct infinite difference obtained from FDTD simulation or PWE needs high-resolution computational grids to resolve the perturbation. Assume that the Wannier functions are found on a computational grid larger than the boundary shift. Because the Wannier functions are continuous and vary significantly only over distances comparable with the wavelength, simple interpolation of the Wannier functions can ensure the accuracy of Eq. (6).

By use of the same method, it is straightforward to show that a dielectric perturbation changes Eq. (3) to $(\mathbf{B} + \gamma\mathbf{D}_{\delta 0}')\mathbf{x} = \mathbf{y}$. It can be shown that, for any invertible matrix, if $\mathrm{d}\mathbf{B}(\gamma)/\mathrm{d}\gamma = \mathbf{D}_{\delta 0}'$, then $\mathrm{d}\mathbf{B}^{-1}(\gamma)/\mathrm{d}\gamma = -\mathbf{B}^{-1}\mathbf{D}_{\delta 0}'\mathbf{B}^{-1}$. Therefore we have a simple expression for the sensitivity:

$$\frac{\mathrm{d}\mathbf{x}(\gamma)}{\mathrm{d}\gamma} = -\mathbf{B}^{-1}\mathbf{D}_{\delta 0}'\mathbf{B}^{-1}\mathbf{y}. \tag{9}$$

Matrix $\mathbf{B}$ is small enough to be inverted directly for structure sizes up to 50 by 50 lattice constants. Therefore $\mathbf{B}^{-1}$ can be obtained when we solve the transmission for the nonperturbed structure, and a change in the transmission–reflection can be determined by use of Eq. (9) with simple multiplication. All the advantages of using $\mathbf{D}_{\delta 0}'$ mentioned above still apply. We refer to both Eq. (7) and Eq. (9) as the WBG method for sensitivity analysis.

We compared the WBG method with direct solution for the perturbed reflection spectrum by use of the FDTD simulation. The test structure and the perturbation are shown in Fig. 1. First we calculated the reflection spectrum for the unperturbed structure using the Wannier basis expansion. The calculation, yielding both the reflection spectrum and the necessary
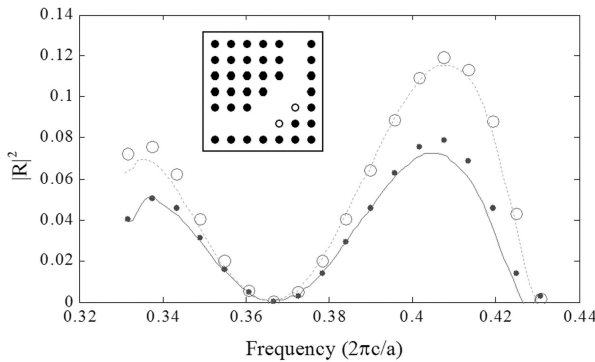
Fig. 1.   Reflection spectra for a PC waveguide bend [see inset: high-index rods ($n = 3.4$) in air, rod radius $0.18a$, where a is the lattice constant].   The two highlighted rods (open circles) in the inset are perturbed by a 10% radius increase. Solid and dashed curves, spectrum from the FDTD method, before and after perturbation, respectively; filled circles, original spectrum found by use of Wannier expansion; circles, perturbed spectrum found by use of Eq. (9).
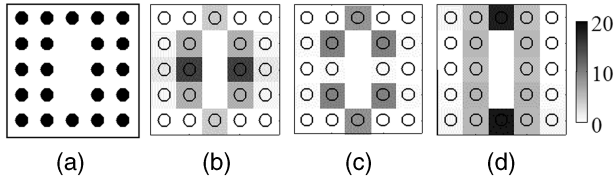

Fig. 2.   (a) Resonator formed by three missing rods.   The computational size is 9 by 9 lattice constants, larger than the area shown.   The PC parameters are the same as in Fig. 1.   (b)–(d) Sensitivity maps for the three eigenfrequencies of the resonator.   The shading above each rod shows the changes to ω in units of $2\pi c/a \times 10^{-4}$ when the particular rod's radius increases by 10%.   Using WBG sensitivity analysis, it took ~10 s to calculate all three maps on a Pentium 3 computer.

matrices for the sensitivity calculation [Eq. (9)], took roughly 30 min on a Pentium 3 personal computer. The result matches well with the FDTD calculation of the spectrum (Fig. 1), which took 10 h on a faster machine.   For the spectrum after perturbation, the WBG result matches well with FDTD calculation (Fig. 1). Another 10 h were needed for this new FDTD calculation.   In contrast, our WBG method took roughly 10 s to compute, since it involves only small matrix multiplications [Eq. (9)].   It should be pointed out that, before the WBG sensitivity analysis, we needed roughly 10 min of computation time to calculate perturbation matrix $\mathbf{D}_{\delta 0}{}'$.   This matrix, however, can be reused if we calculate the perturbed spectrum that results from a 10% radius increase for any other rod or rods in any device constructed with the same PC.   Each additional spectrum will then be obtained in a matter of seconds.

We also verified the WBG sensitivity calculation for a PC defect resonator by use of PWE.   The structure is shown in Fig. 2(a).   First, a Wannier expansion calculation yields resonator eigenfrequencies and the vectors needed for the sensitivity calculation [Eq. (7)].

When found this way, ω agrees with PWE calculations to four significant figures.   Then, the rod at row 3, column 2 in Fig. 2(a) is perturbed by a 10% radius increase.   Three methods were used to find the changes ($\Delta\omega$) for the three eigenfrequencies.   Using PWE directly to find ω of the perturbed structure took ~2 h, and $\Delta\omega$ were found to be 1.35×10^{-3}, 5.20×10^{-5}, and 6.87×10^{-4}.   Because adding a perturbation is no different from changing the resonator design, we can solve the new values of ω directly, using the Wannier expansion again.   This took ~1 min ($\Delta\omega = \{1.34 \times 10^{-3}, 5.10 \times 10^{-5}, 5.91 \times 10^{-4}\}$). The WBG method, using Eq. (7), took less than 1 s ($\Delta\omega = \{1.52 \times 10^{-3}, 4.48 \times 10^{-5}, 4.76 \times 10^{-4}\}$).   Discrepancies among the three methods are less than 15% for the first two modes.   The highest frequency mode is very close to the band edge of the PC, so the result from PWE is less reliable.   The error in the WBG method is due to the fact that we used only a linear projection to approximate $\Delta\omega$ based on the slope found in Eq. (7).

As we have shown, even without using Eq. (7), solving for $\Delta\omega$ directly in the Wannier basis already offers a large increase in speed over PWE.   To demonstrate the advantage of using WBG over rerunning the Wannier expansion, we calculated $\Delta\omega$ as a result of a 10% radius change for each and every rod in the resonator.   The results for all three modes are shown in Fig. 2.   Because Eq. (7) is a simple multiplication, the three sensitivity maps took a total of 10 s to calculate. Solving for $\Delta\omega$ directly in the Wannier basis requires solving a separate matrix eigenvalue equation for each lattice site and will take more than 1 h.   If we use PWE, more than 100 h will be needed.   Therefore, if we need to search through a large number of designs for a given sensitivity criterion, using the WBG approach is the only practical method available that is known to the authors.

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References

1. A. Taflove and S. C. Hagness, *Computational Electrodynamics: the Finite-Difference Time-Domain Method*, 2nd ed., Artech House Antennas and Propagation Library (Artech House, Norwood, Mass., 2000).
2. S. G. Johnson and J. D. Joannopoulos, Opt. Express **8,** 173 (2001), http://www.opticsexpress.org.
3. G. Veronis, R. W. Dutton, and S. Fan, Opt. Lett. **29,** 2288 (2004).
4. J. P. Albert, C. Jouanin, D. Cassagne, and D. Bertho, Phys. Rev. B **61,** 4381 (2000).
5. D. M. Whittaker and M. P. Croucher, Phys. Rev. B **67,** 085204 (2003).
6. K. Busch, S. F. Mingaleev, A. Garcia-Martin, M. Schillinger, and D. Hermann, J. Phys. Condens. Matter **15,** R1233 (2003).
7. S. G. Johnson, M. Ibanescu, M. A. Skorobogatiy, O. Weisberg, J. D. Joannopoulos, and Y. Fink, Phys. Rev. E **65,** 066611 (2002).
8. R. A. Horn and C. R. Johnson, *Matrix Analysis* (Cambridge U. Press, Cambridge, England, 1990), p. 561.