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Theoretical Prediction of Thermooptical and Structurally Disordered Sensitivities in Metallo-Dielectric Photonic Crystals

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Abstract—In this letter, we introduce a novel computational technique for predicting thermal and structural sensitivities in metallo-dielectric photonic crystals (PCs). The computational scheme is based on a hybrid formalism of the scattering matrix technique combined with the adjoint network method. The proposed technique can predict with high accuracy the impact of temperature fluctuations or structural disorders, to the light-wave propagation in PCs, without additional computational effort. Numerical simulations show that PC circuits based on metallic-metamaterial platforms are significantly less sensitive to temperature variations in comparison to usual dielectric PCs.

Index Terms—Lightwave propagation, metamaterials, photonic crystal (PC) circuits, sensitivity.

I. INTRODUCTION

PHOTONIC crystals (PCs) have recently attracted considerable attention by optical scientists, because they can radically alter the optical properties of matter in an extraordinary way [1].

In practical realization of PC devices, it is of fundamental importance to accurately predict the sensitivity of the device properties to fabrication tolerances. Sensitivity analysis of environmental temperature fluctuations is also important, especially for characterizing the thermal stability of PC devices, and can be particularly helpful in deciding whether to use a special temperature maintaining environment to stabilize transmission. Until recently, however, such sensitivity studies have been reported only for structural disorders, and in particular for PCs composed of usual dielectric materials [2]–[5].

The inclusion of metals in PCs, operating at optical wavelengths, has attracted significant attention due to their surprising ultralow refractive index metamaterial characteristics [6], [7]. However, the sensitivity properties of metallic PC metamaterials have not been reported so far, mainly for two reasons. First, a general technique which permits the calculation of both structural and temperature sensitivities was not known. Second, for the optical characterization of metallic materials, a simplified temperature-independent Drude model has been used so far [8], thus prohibiting the thermal properties of these nanocomposites to be studied. Taking all the above circumstances into account, in this letter, we describe a novel sensitivity analysis technique based on a hybrid formalism of the scattering matrix method [9]–[11] with the adjoint network method [12], [13], for performing fast and accurate sensitivity calculations in PCs. Such an analytical technique which permits the study of both structural and temperature fluctuations in PCs will be reported for the first time. In particular, we show through numerical simulations that the use of metallic metamaterial PCs significantly reduces the sensitivity to temperature fluctuations in comparison to usual dielectric PCs.

II. HYBRID COMPUTATIONAL SCHEME FOR CALCULATING SENSITIVITIES IN PCs

In the standard analysis of PC circuits using the scattering matrix technique [9]–[11], we arrive at a matrix equation for the unknown expansion coefficients for the field distribution $B_j$, $j = 1, 2, \ldots, N$, where $N$ is the total number of cylinders in the PC under consideration, which has the following form:

$$
\begin{bmatrix}
I & -S_1 T_{1,2} & \cdots & -S_1 T_{1,N} \\
-S_2 T_{2,1} & I & \cdots & -S_2 T_{2,N} \\
\vdots & \vdots & \ddots & \vdots \\
-S_N T_{N,1} & -S_N T_{N,2} & \cdots & I
\end{bmatrix} \begin{bmatrix}
B_1 \\
B_2 \\
\vdots \\
B_N
\end{bmatrix}
= \begin{bmatrix}
S_1 Q_1 \\
S_2 Q_2 \\
\vdots \\
S_N Q_N
\end{bmatrix}
$$

(1)

where $I$ denotes the unit matrix, and $S_j T_{jk}, Q_j$ are quantities defined explicitly in terms of Hankel and Bessel functions for $j = 1, 2, \ldots, N$, and $k = -N, \ldots, +N$ and can be found in [9] and [11]. Using standard notations from the method of moments, we can rewrite (1) in the following compact form:

$$
\mathbf{\mathcal{Z}}(\mathbf{x}) \cdot \mathbf{\mathcal{B}} = \mathbf{\mathcal{F}}.
$$

(2)

Here, $\mathbf{x}$ is the vector of design parameters, $\mathbf{\mathcal{B}}$ is the state vector with the unknown coefficients of the field distribution, $\mathbf{\mathcal{F}}$ is the global excitation vector which carries the information of the source excitation and the Sommerfeld radiation condition at infinity, and $\mathbf{\mathcal{Z}}(\mathbf{x})$ is considered to be a nonsingular interaction matrix which carries all the information for the structural and material properties of the PC under consideration. Thus, we restrict our analysis in PCs with low coupling between the waveguide channel and coherent cladding modes. A global objective function which can be any electromagnetic quantity (e.g., transmission characteristics in which we want to calculate the sensitivity response) that is differentiation with respect to the design parameter $\mathbf{x}$, is defined explicitly as $f(\mathbf{x}, \mathbf{\mathcal{B}}(\mathbf{x}))$. From
model the material characteristics of metallic nano-pillars, we have adopted a temperature-dependent Drude model [14]
\[ \varepsilon_{\text{metal}} = 1 - \varepsilon_\infty \left( \frac{\omega_p^2 + \nu_c^2}{\omega^2} + j \varepsilon_\infty \frac{\omega_p^2 + \nu_c^2}{\omega^2} \frac{\nu_c}{\omega^2 + \nu_c^2} \nu_c(\omega, T) \right) \]
\[ = \nu_{\text{d}} \left[ 1 + \left( \frac{\hbar \omega}{2 \pi k_B T} \right)^2 \right] \]  
where \( \varepsilon_\infty \) is the relative dielectric constant at high frequencies, \( \omega_p/(2\pi) = 2175 \) THz is the plasma frequency, \( \nu_{\text{d}}/(2\pi) = 4.35 \) THz is the classical relaxation rate in the free electron model of metals, \( \omega \) is the angular frequency, \( T \) is the absolute temperature, \( k_B \) is the Boltzman’s constant, and \( \hbar \) is the Plank’s constant. The above parameters correspond to silver (Ag) which will be considered as a model metal. In the case of usual dielectric materials, we consider the following Drude–Lorentz type of dielectric permittivity [15] of intrinsic semiconductors
\[ \varepsilon(\omega, T) = \varepsilon_d \left[ 1 - \frac{\omega_p^2(T)}{\omega^2} \right] \]  
\[ \omega_p^2(T) = \sum_i \frac{4\pi n_i e_i^2}{m_i c_d} n_e(T) = 5.76 \times 10^{14} T^{3/2} \exp \left( \frac{-0.13}{k_B T} \right) \]  
where \( \varepsilon_d = 17.7, n_e/m_e = 0.015, n_e \) is the density of the free electrons and holes in the relevant conduction (\( i = e \)) and valence band (\( i = v \)), and \( m_i/m_e \) stands for their effective masses. These parameters correspond to the intrinsic semiconductor known as InSb. In our investigations, however, we will also consider the case of GaAs, which has larger electronic band-gap. Additionally, we assume that the geometrical characteristics of the pillars will remain invariant as the temperature changes and only the permittivity function is affected.

A. Validation of the Proposed Computational Scheme

In order to validate our computer code, we perform a comparison with already reported calculations of structural sensitivities in usual semiconducting PCs (GaAs rods in air). Following the example of [2, Fig. 13], Fig. 2 shows the results obtained with our method (solid line) and the finite-element method used in [2] (dotted line). We can clearly see that there is a good agreement between the two methods, a fact that ensures the accuracy and the efficiency of our computer code.

B. Computation of Structural and Thermal Sensitivities

To demonstrate the calculation of structural sensitivities (first-order derivative of the global objective function with respect to the design parameter) of the device in Fig. 1, we consider as a global objective function the transmission characteristic \( T_0(\omega, \Delta R) = P_{\text{OUT}}/P_{\text{IN}} \), at constant temperature \( T_0 = 300 \) K, and as a vector of design parameters the single scalar variable \( \Delta R \), which is the perturbed portion of the radius of the single defect, as shown in Fig. 1. The upper panel in Fig. 3 shows the sensitivity of the transmission curve as a function of the normalized perturbation \( \Delta R/R_0 \), for dielectric-InSb (dotted line), or metallic-Ag nanopillars (solid line). From these results, we can conclude that the dynamic rate of change
in the transmission curve, namely the difference between local minima and maxima of the sensitivity curve is greater in case of the metallic-defect, than that of the dielectric, especially for higher tolerances (13%–30%). The physical explanation for this result is that the metallic nanowires interact more strongly with light, in the visible and near-infrared frequency bands, and as a result they are found to have more pronounced reflectivity. As a consequence, a high structural variation of the metallic nanowires, especially in the case where they are positioned near discontinuities of waveguide bends, will result as a general rule in larger sensitivities than the case of dielectric defected nanowires. The lower panel in Fig. 3 demonstrates the calculation of thermal sensitivities (first-order derivative of the global objective function with respect to the temperature), at a frequency-\(\omega_2\) corresponding to maximum transmissivity, in case of \(\Delta R = 0\). The calculation is performed for silver (Ag), and for semiconducting materials, InSb (dotted line) and GaAs (dashed line). From these results, we can clearly see that the metallic-based platform is less sensitive to thermal fluctuations. In addition, we conclude that semiconductors with a larger electronic bandgap (GaAs) exhibit lower sensitivity in comparison to semiconductors with a smaller electronic bandgap (InSb). Even in such cases, the sensitivity of the metallic platform is at least two to five times smaller than that of GaAs, over a wide range of temperatures.

### IV. CONCLUSION

An efficient analytical computational scheme for fast and accurate predictions of thermal and structural sensitivities in metallo-dielectric PCs has been proposed. We have demonstrated that metallic-based metamaterial PCs are less sensitive to temperature variations than usual PCs based on dielectric platforms. A generalized stochastic method for yield analysis in PCs with random structural disorders is currently under consideration.

### REFERENCES