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Design of Si–SiO₂ Phoxonic Crystal Having Defect Layer for Simultaneous Sensing of Biodiesel in a Binary Mixture of Diesel Through Optical and Acoustic Waves¹

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Abstract— The potentiality of a phoxonic crystal for sensing of biodiesel in a binary mixture of diesel and biodiesel is theoretically investigated. Using the transfer matrix method, the transmission of acoustic and optical waves through a periodic one-dimensional crystal of $Si-SiO_2$ layers is studied. A pass band is created in the band gap region by introducing a cavity in the considered one-dimensional crystal structure. This pass band can also be considered as a defect mode, and it is found that its position is highly dependent on mole concentration of binary mixture of biodiesel and diesel present in the cavity. The sensitivity of the sensor for a binary mixture of biodiesel and diesel in the cavity with various mole concentrations is estimated. Simulated results provide a valuable guidance for designing a phoxonic crystal sensor consisting of a defect layer.

Keywords: phoxonic crystal, defect layer, sensitivity, biodiesel sensor **DOI:** 10.1134/S1063771017020117

1. INTRODUCTION

Environmental concerns, global climate change and energy security for future have stimulated worldwide interest in biofuels. Biodiesel is typically made by chemically reacting lipids (e.g., vegetable oil, animal fat) with an alcohol producing fatty acid esters. Materials like corn and soybeans have oil extracts that can be converted to ethanol or biodiesel [1]. Biofuels are used as an additive (B20 where 20% of the mixture consists of biodiesel and 80% regular diesel) with diesel to reduce vehicle emissions or in its pure form as a renewable alternative fuel for diesel engines. Biodiesel fuel can limit the amount of harmful emissions. Even a lower mixture such as B20 has a tremendous impact on the environment [2]. Biodiesel is an economic alternative, especially for compression ignition engines, because it is a renewable energy source that can be used in these engines without significant changes in their design. Fuel producers have developed some standards for biodiesel, such as EN 14214 and ASTM D 6751, in close cooperation with car, engine and injection pump manufacturers [3]. Hence mixing of biodiesel in diesel is an important issue for fuel producers to satisfy the standards for biodiesel. Therefore, in the present communication a novel method for monitoring of biodiesel through phoxonic crystal sensor in a binary mixture of diesel is proposed.

Phoxonic crystals are crystal that show the phononic and photonic band gaps simultaneously. Phononic crystal and their optical complement, so called photonic crystals, are well known for their ability to control the propagation of guided acoustic and optical waves [4–6]. Any change in the building block of the crystal shows changes in the transmission properties of the crystal, and the measurement of these changes gives a concept of photonic and phononic sensors [7, 8]. For the optical case the key parameter is the refractive index, and in the acoustic case it is density or sound velocity. There are many research papers on sensing applications showing the capability of phononic and photonic crystals for detecting small variations in density and refractive index respectively. A possibility to determine the octane number of gasoline through a liquid filled slit cavity mode in phononic and photonic crystals for a sensitive microscale chemical and biochemical sensing is presented by many groups of researchers [9, 10]. A phoxonic crystal sensor allows a dual parallel determination of two independent material properties by combining both concepts in one device [11]. To enhance the optomechanical interaction a defect has been introduced to create a cavity trap for both phonons and photons by using the simultaneous existence of phononic and photonic

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Fig. 1. Structure of the 1D phoxonic crystal with a cavity.

band gaps [12]. In contrast, the correlation between the material parameters like the speed of sound and speed of light and frequency of cavity modes confined in the cavity is the basic idea behind the application of phoxonic crystals as a sensor platform. Transmission of frequency in the band gap is related to several parameters of practical interest like concentration of one component in a mixture or conversion rate in the cavity. The sensing phenomenon is based on the highly sensitive localized modes for variation in refractive index, density and velocity of sound waves in a fluid. These modes are associated with defects and appear inside the band gap. In this regard, our aim is to emphasize the potentiality of phoxonic crystal for a sensing platform with dual characteristic (acoustic and optical waves) investigation in the same structure. Hence, in the present paper, both acoustic and electromagnetic field with well confinement of cavity mode propagation in Si-SiO₂ periodic structure without substrate are discussed in details. These defect modes give rise to peak in transmission band that are sensitive to the material filled in cavity. The geometrical parameters of the sensor are discussed such as to define a dual band gap sensor. The transfer matrix method was employed to obtain the transmittance and to study the effect of fluid in cavity on the pass band. The dependency of the pass band on molar ratio of biodiesel and diesel present in cavity is investigated.

2. THEORETICAL MODELLING

A schematic diagram of the considered one dimensional (1D) phoxonic crystal structure is shown in Fig. 1. The phoxonic crystal is composed of periodically alternating layers of Si and SiO₂ with thicknesses d_1 and d_2 respectively. A cavity of thickness d_c is positioned in the middle of the periodic structure as a defect layer. The considered 1D phoxonic crystal has a mirror symmetry about the cavity and there are seven unit cells on each side. The transfer matrix method to study the acoustic wave and optical wave propagation in a 1D phoxonic crystal with a cavity is applied. One unit cell of the crystal is composed by one layer of Si and SiO₂ with dielectric functions ε_1 , ε_2 , densities ρ_1 , ρ_2 and longitudinal velocities v_1 , v_2 respectively. The propagation of the wave in 15 layers with one defect layer in a one-dimensional Si-SiO₂ structure with period parameters $n(z) = n(z + \Lambda)$, $\rho(z) = \rho(z + \Lambda)$ and $v(z) = v(z + \Lambda)$ of the period $\Lambda = a = d_1 + d_2$ is considered.

The pressure of the normally incident longitudinal elastic wave propagating through the phoxonic crystal from the left to the right in a medium is governed by the following wave equation:

$$\frac{1}{v_n^2} \frac{\partial^2 p}{\partial t^2} - \nabla^2 p = 0.$$
 (1)

Here v_n is the elastic wave velocity in the n^{th} layer of the crystal structure. The 1D plain wave solution of this equation in given by

$$p_i = A_n e^{i(\omega t - k_1 x)} + B_n e^{i(\omega t + k_1 x)} \quad 0 < x < d_1,$$
(2a)

$$p_i = C_n e^{i(\omega t - k_2 x)} + D_n e^{i(\omega t + k_2 x)} d_1 < x < \Lambda,$$
 (2b)

 $k_1 = \omega \sqrt{\rho_1/c_1}$ and $k_2 = \omega \sqrt{\rho_2/c_2}$, where ω is the angular frequency, c_1, c_2 are shear elastic stiffnesses of silicon and silicon oxide respectively. The first and second terms of the right side in equations (2a, 2b represent the forward and reflected waves respectively. The wave function and the shear stress must be continuous at the Si–SiO₂ interface leading to the following relations among the coefficients A_n , B_n , C_n , and D_n in the n^{th} cell:

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \frac{1}{2z_1} \begin{pmatrix} (z_1 + z_2) e^{i(k_1 - k_2)(n\Lambda - d_1)} & (z_1 - z_2) e^{i(k_1 + k_2)(n\Lambda - d_1)} \\ (z_1 - z_2) e^{-i(k_1 + k_2)(n\Lambda - d_1)} & (z_1 + z_2) e^{i(k_1 + k_2)(n\Lambda - d_1)} \end{pmatrix} \begin{pmatrix} C_n \\ D_n \end{pmatrix} = M_{n\Lambda - d_1} \begin{pmatrix} C_n \\ D_n \end{pmatrix}.$$
(3)

Similarly, we can write a relation between the coef-ficients C_n , D_n and A_{n+1} , B_{n+1} for adjacent cells:

$$\begin{pmatrix} C_n \\ D_n \end{pmatrix} = \frac{1}{2z_2} \begin{pmatrix} (z_1 + z_2) e^{i(k_2 - k_1)n\Lambda} & (z_2 - z_1) e^{i(k_2 + k_1)n\Lambda} \\ (z_2 - z_1) e^{-i(k_2 + k_1)n\Lambda} & (z_1 + z_2) e^{i(k_2 + k_1)n\Lambda} \end{pmatrix} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = M_{n\Lambda} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix},$$
(4)

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