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Anna Baldycheva
Trinity College Dublin

Vladmir A; Tolmachev
Ioffe Physico-Technical Institute

Tatiana S. Perova
Trinity College Dublin

See next page for additional authors

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Authors

Anna Baldycheva, Vladimir A. Tolmachev, Tatiana S. Perova, and Kevin Berwick

Formation of infrared windows of transparency in one-dimensional silicon photonic crystals

Anna Baldycheva¹, Vladimir A. Tolmachev², Tatiana S. Perova^{1,*} and Kevin Berwick³

¹*Department of Electronic and Electrical Engineering, Trinity College Dublin, Dublin 2, Republic of Ireland*

²*Ioffe Physical Technical Institute, Polytechnicheskaya 26, St. Petersburg, Russian Federation*

³*Department of Electronic and Communications Engineering, Dublin Institute of Technology, Kevin St, Dublin 8, Republic of Ireland*

*perovat@tcd.ie

Abstract: In this study, three-component One-Dimensional Photonic Crystal (1D PC) structures were investigated by modeling them as two-component PCs with an additional regular layer. The Gap Map approach and the Transfer Matrix Method were used in order to mathematically describe these structures. The principle of suppression of the reflection bands and replacing them with regions of transparency is demonstrated for a high contrast 1D PC for the first time. The regions of transparency obtained show a high transmission value (>0.99) and a substantial band width in the infrared spectral range.

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1. Introduction

Photonic Crystals (PCs) [1,2] have attracted considerable scientific and commercial interest in recent decades because of their unique properties in manipulating light. Photonic Crystals exhibit total reflection over a range of frequencies, that is, they have a Photonic Band Gap (PBG). Optical devices based on multi-dimensional PCs can be used to fabricate numerous optical elements, including waveguides, reflectors, attenuators of spontaneous atomic emission and devices for controlling emissions in micro-cavities [1-3]. These devices operate by the PBG effect and, therefore, possess high sensitivity to the refractive indices, N , of their components. Manipulation of N allows the design of PBG materials whose optical characteristics can be varied over a wide range. The PCs are normally composed of only two-components, with high (N_H) and low (N_L) refractive indices. However, some recent studies have explored the optical properties of multi-component 1D and 2D PCs [5,6]. The authors of Ref.[6] have shown, based on an example of 2D PCs, a shift of the band gaps' edges. This shift depends on the thickness and dielectric constant of the intermediate layer on the surface of the cylindrical pores. The authors attribute the shift as being due to a decrease in the effective dielectric constant of the system. The authors of a different paper [7] studied a multi-component model for a more complex, 3D PC structure, and have shown, based on an opal structure example, that it is possible to selectively manipulate the PBGs in this PC.

In our previous paper [8], we selected a 1D PC, based on grooved silicon, as the simplest illustrative example for calculations and fabrication. This structure demonstrates PBG modification, in both position and width, when an additional, regular t-layer is introduced to the PC. The addition of this regular t-layer transforms the original, two-component PC into a three-component PC. Manipulation of the optical contrast of the original two-component PC is achieved, not by filling its air channels with a liquid or solid, but by the selection of the thickness or the refractive index of the additional t-layer, the third component.

We have found that the introduction of the additional layer with a specific optical thickness can, under some conditions, result in the disappearance of the PBGs in the Gap Map (GM) [8]. A similar effect has already been observed for periodic, multilayer filters [16, 17]. The authors of Refs. [16,17] presented a specific set of design criteria which will cause the position of the high- and low-transmission bands in the transmission spectrum to be shifted. More recent studies have been performed [18] for multi-component dielectric coatings in the near infrared (NIR) region. In the present paper, we extend this approach i) by using a periodic structure with high-optical contrast, viz. "Si-air" and ii) by generating maps of regions of transparency or Transmission Bands (TBs), for the first time.

2. Results and discussion

2.1 Modeling of three-component photonic crystal structure

A periodic Si structure with linear grooves on a micro scale¹⁹ is considered here as a model for a 1D PC structure. The refractive index of Si, $n_{Si} = n_H = 3.42$ is used for the high-refractive index, H , component, while the refractive index of the air grooves for the low-refractive index, L , component is taken as $N_{air} = N_L = 1$. This results in the refractive index contrast $\Delta n = 3.42/1$ and the resulting PC can be considered as a high-optical contrast photonic crystal. Therefore only a small number of periods, m , are needed in order to obtain a PBG with a reflectance of over 0.999. We take the number of periods as $m=5$. We would like to investigate the impact on the PBGs caused by the insertion of an additional regular layer, known as the t -layer, with refractive index, n_t , values between 3.42 and 1. For example, an SiO₂ interlayer, with a refractive index $n_t = 1.5$, can be deposited on the Si walls of the 1D PC structure with a specific lattice constant, A [6].

Reflection, R , spectra of 1D PCs were calculated using the Transfer Matrix Method (TMM) [20]. This method is attractive due to the ease of introduction of an arbitrary number of additional layers at any point in the TMM's equation. Utilization of the GM presentation gives a visual representation of the transformation of PBG areas during the transition from a two-

component to a three-component PC. Note that all the optical characteristics presented in this study have been simulated for a normal incidence of light and $N=1$ for the incoming and outgoing media. We use normalized frequency, $NF=A/\lambda$, units and, therefore, the results obtained can be applied to a wide range of structure sizes, including micro- and nano-structures.

An analysis of the GMs of the lowest PBGs for the three-component PC revealed a red shift, as well as a decrease of the PBG area, with respect to the original two-component PC, with an increase of the t -layer thickness, D_t [8]. Similar behavior has been observed in the GM of PBGs for a two-component PC with increasing N_L [10]. Thus, introduction of the t -layer has a similar effect to the substitution of N_L , i.e. it serves to decrease the optical contrast or, in accordance with Ref. [12], to decrease the effective dielectric constant. Changing the refractive index, N_t , is an alternative method of modifying the optical contrast and, like D_t , the value of N_t can be altered technologically. So, by changing the values of $D_t N_t$ for the t -layer in a multi-component structure, new types of PC structures with optical contrasts from 3.42/1 to 3.42/1.5 can be designed.

Fig.1. GMs for a two-component PC with optical contrast $N=3.42/1.1$ (grey line) and for three-component PC with $N_t=1.5$ and $D_t=0.13A$ (black line) over a range of NF .

As discussed in our previous paper [1], a three-component PC with an optical contrast, Δn_1 can be considered equivalent, to a first approximation, to a two-component PC with a different optical contrast, Δn_2 . In this study, we calculated the GMs for a two-component PC with $N_L=1.1$, equivalent to a three-component PC with $N_t=1.5$ and $D_t=0.4A$. The GMs obtained for both of these PCs are presented in Fig. 1 for a wide range of NF . It is apparent from Fig. 1, that the range of possible filling fractions, f_{Si} , required for the formation of PBGs is reduced to below a specific value of f_{Si} . The limit placed on the value of f_{Si} is due to the fact that the value of D_L decreases as a result of the introduction of the t -layer of thickness D_t [SPIE2009].....The larger the value of D_t , the lower the maximum value of the filling fraction f_{Si} that can be realized in the three-component PC (see also Section 2.2). It is also apparent that the lower PBGs are the least affected by the addition of the new layer, retaining a similar area and experiencing a negligible shift in frequency. Examination of the high-order PBGs, shown in Fig. 1, for the three-component PC over the entire range of NF , reveals regions of frequency, or equivalently wavelength, for which PBGs are suppressed, with $R<0.999$. Note that the PBGs determined for the equivalent two-component PC structure are not suppressed over the entire NF range (Fig.1, marked as 1.1).

Calculations of the reflection spectra of the three-component PC structure investigated for selected values of f_{Si} have shown significant suppression and, in addition, a disappearance of the reflection bands ($R=0$) in certain regions of NF . It is obvious that these NF regions could be replaced by regions of transmission instead; however it is not clear what the maximum values of T would be and what the width of the transmission range might be. In order to answer this question, an analysis of the transmission spectra is performed in the next Section.

2.2 Formation of regions of transparency in a three-component photonic crystal structure

A set of transmission spectra was calculated for a three-component 1D PC with a t -layer thickness of $D_t=0.1A$ over a range of f_{Si} values from 0.08 to 0.01 with a step size of 0.003 (Fig. 2(a)). Obviously, the transmission bands (TBs) are formed between suppressed PBGs, with R less than 0.999. It is clear from Fig. 2(a) that the TB's range is constant for a fixed optical

thickness of the additional layer $D_f N_f$, as well as for the filling fraction, f_{si} , in the range 0.083 to 0.093, that is, with a change in the filling fraction of $\Delta f_{si}=0.093-0.083=0.01$. Additional detail can be seen on Fig. 2 (b), where the transmission range is expanded across the range of transmissions from 0.97 to 1 in order to increase the clarity of the diagram. As shown in Fig. 2(b), the width of the TBs is also dependent on the selection of the cutoff transmission value. For example, if a cutoff transmission was chosen as 0.995, then the TBs within a narrow range of normalized frequencies will appear narrower and less uniform than those for a cutoff level of 0.99. Choice of an appropriate cutoff level is an important design criterion when engineering practical device structures.

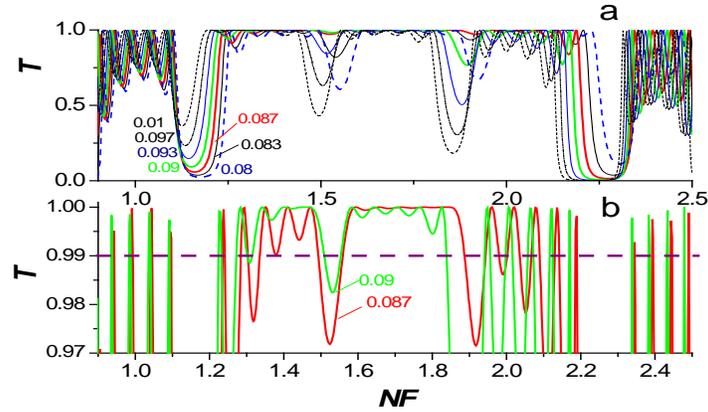
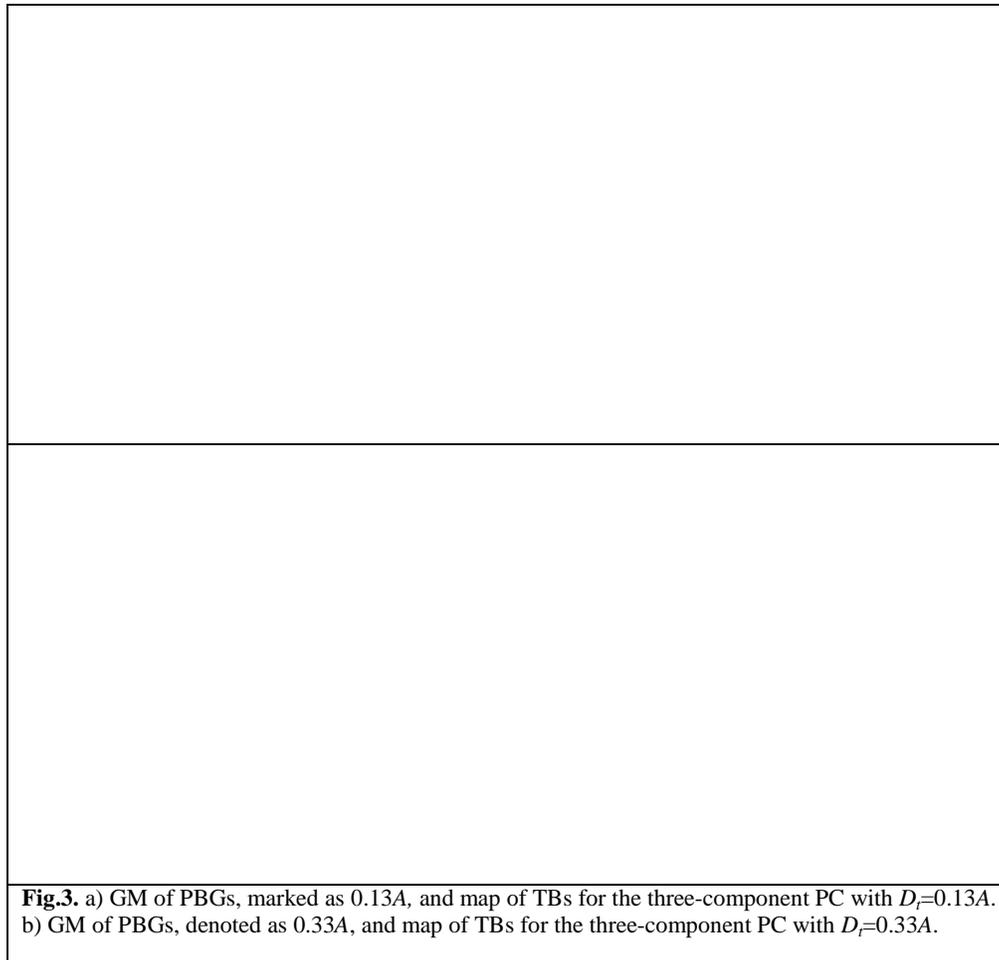


Fig.2 Transmission spectra T for three-component PC (a) detail from the spectra with expanded transmission scale (b). $N_f=1.5$, $D_f=0.1A$. Numbers beside spectra correspond to f_{si} values.

The second criterion for TB formation is the selection of the minimum range of $\Delta NF > 0.01$, which provide transmission values $T > 0.99$. This enables us to remove narrow peaks of high transmission, $T > 0.99$, from the spectrum in Fig. 2(b) (see, for example, peaks at $NF=1, 2.1, 2.4$). Removal of these regions greatly improves the clarity of the TBs in Fig. 3. It can be also seen from Figure 2, that TBs can appear in a very narrow range of f_{si} values, so these calculations must be performed using a small step size, Δf_{si} . A step size of $\Delta f_{si}=0.01$ was used for this study.

Now that we have established the general criteria for TB formation, we can plot a map of the regions of transparency for the three-component PC, as shown in Fig. 3(a). As expected, the TB regions are located between the PBG areas of the corresponding PC structure. Note the total suppression of high order PBGs over a range of NF . This NF range also contains the widest TBs. The range of frequencies over which the high-order PBGs are suppressed and replaced by TBs over a range of filling fractions f_{si} (Fig.3(a)) is denoted the Window of Transparency (WT). Therefore, we conclude that the third layer in the PC structure can be treated as an antireflection layer by analogy with multilayer dielectric coatings.

We then calculated the TB maps for a three-component PC with t -layer thicknesses ranging from $0.2A$ to $0.47A$ with a step size of $0.07A$ in order to analyze the changes that occur in the WTs when the thickness of the additional t -layer is varied. The calculation procedure used to determine the TBs and their graphical representation is the same as that described earlier for creating the GM for PBGs [Appl.Opt.].



It is worth noting that, even for the PC with $D_t=0.20A$, the TBs exhibit a different behavior to that for the case of $D_t=0.13A$. The TW disappears, reappearing again in two NF regions. Moreover, with an additional layer thickness of $D_t=0.33A$, we can observe the emergence of three TWs over the same NF range (Fig 3(b)). Thus, an increase in the t-layer thickness results in an increase in the number of TWs.

These preliminary calculations allowed the impact of varying the additional layer thickness on WT formation to be determined. As pointed out earlier, a variation in the thickness of the additional layer can change the optical contrast of the structure, changing both the position and number of WTs. Consequently, TB narrowing and damping of the WTs will occur over the entire frequency range. The effect, demonstrated here, of suppression of the photonic band gaps and their replacement with regions of transparency, has practical applications in integrated silicon micro-photonics. It suggests that fabricating interference filters with nearly 100% transmission over selected ranges of the infrared spectrum is practical.

3. Conclusion

In this paper, the optical properties of three-component 1D PC structures were investigated by modeling them as two-component PCs with an additional regular t -layer. The Gap Map approach and the Transfer Matrix Method were used in order to mathematically describe these PC structures. It was found that the introduction of the t -layer affects the properties of high-order PBGs, replacing them with transmission bands and creating windows of transparency over certain frequency, or equivalently wavelength, ranges. By varying the thickness of the t -layer, the width and the number of the windows of transparency can be altered. A map of the transmission bands for a three-component photonic crystal was generated for the first time. This map constitutes a unique design tool for infrared optical filters based on three-component Si photonic crystals. We note that the approach suggested can also be applied to the design of any microstructured semiconductor or dielectric materials for application across the entire electromagnetic spectrum.

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