

Optical characteristics of a one-dimensional photonic crystal with an additional regular layer

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ABSTRACT

In this paper, the forbidden Photonic Band Gaps (PBGs) of a one-dimensional Photonic Crystal (1D PC) with additional regular layer, t for the constant value of the lattice constant A and at normal incident of light beam were investigated. The additional regular layer was formed from both sides of the high-refractive index layer H . The gap map approach and the Transfer Matrix Method were used for numerical analysis of this structure. The limitation of filling fraction values caused by the presence of t -layer was taking into account during calculations of the Stop-Band (SB) regions for three-component PC. The red shift of SBs was observed at the introduction of t -layer to conventional two-component 1D PC with optical contrast of $N=3.42/1$. The blue edge of the first PBG occupied the intermediate position between the blue edges of SBs regions of conventional PCs with different optical contrast N . This gives the opportunity of tuning the optical contrast of PC by introduction of the additional layer, rather than using the filler, as well as fine tuning of the SB edge. The influence of the number of periods m and the optical contrast N on the properties of SBs was also investigated. The effect of the PBG disappearance in the gap map and in the regions of the PBGs of high order was revealed at certain parameters of the additional layer.

Keywords: 1D Photonic Crystal, Tunable Photonic Crystal, Multicomponent Photonic Crystal, Photonic Gap Map

1. INTRODUCTION

New areas of research in micro photonics have been opened up due to developments in the theory and application of photonic crystals (PCs). Photonic crystals possess unique optical properties and can be used as reflectors, attenuators of the spontaneous atomic emission, devices for controlling emission in micro cavities, waveguides and others¹⁻⁴. One dimensional (1D) PCs are normally composed of two components with high (N_H) and low (N_L) refractive indices and two geometrical thicknesses D_H and D_L , accordingly. The examples of 1D PCs are the multilayer films obtained by various methods of deposition onto different substrates and micro-structured semiconductors such as the combination of Si layers with different porosity or grooved Si⁴. If some additional t -layer exists between the high (H) and the low (L) refractive index components for all interfaces of 1D PC, this layer can be considered as an additional regular structure (Fig.1) in PC thus making this PC a multi-component photonic structure.

Multi-component PCs have already been investigated in a number of recent papers, among which it is worthwhile to refer to the investigation of multi-component 1D PC^{5,6}. The authors of paper⁵ have analyzed the relation of photonic band-gap (PBG) property with the arrangement of components, the refractive index and the geometrical thickness. However the same geometrical thickness was used for all the layers in a structure despite the fact that it is well known that the thickness of each PC component significantly influences the optical properties of photonic crystal. The authors of Ref.⁶ have investigated theoretically and experimentally how the additional layer, introduced between H - and L -component, can influence the reflectance spectrum position and leads to the narrowing of high-order band gap. As a result the analysis, performed in Refs.^{5,6}, is related to specific structural types only and does not reflect the general behavior of multi-component PCs.

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In paper⁷ more detailed investigations of 2D photonic crystals, containing intermediate layers on the surface of cylindrical pores, have been carried out. The authors have obtained the dependences of the PBG width and position on the additional interlayer thickness and its dielectric constant. They have considered a possibility to vary the lowest band gap position and its width in 2D photonic crystals contained interlayer. It was shown that an interlayer with a thickness of only $d = 0.01A$ influences the band gap position quite significantly. In addition the insertion of the third component into the photonic structure decreases the PC's contrast and, consequently, the band gap width. The authors of Ref.⁷ have also examined the behaviour of the lowest PBG for a small range of filling fractions which are optimal for the PBGs formation for studied 2D PC.

The authors of paper⁸ succeeded in studying multi-component 3D PC and have shown how to selectively manipulate with stop-bands in multi-component photonic crystal based on opal structure. For the description of optical characteristics with respect to the structural features more complicated model approaches, than that for 1D and 2D structures, were used. They have shown the possibility to control the stop-bands appearance, their width, shift and ON/OFF switching by variation of t -layer thickness, permittivity and other factors in multi-component PC.

In the present paper, we have selected the 1D PC as the most simple example from the point of view of calculation, as well as for the demonstration of ON/OFF effects and stop bands modifications (in position and width) due to the introduction of an additional regular t -layer with variations of the thickness and the refractive index of t -layer as well as the filling fraction and the optical contrast of two-component PC. We have analyzed the construction of the PCs Stop-Bands (SBs) for three-component PC structure based on the Gap Map (GM) approach^{3,9}. As was already shown in the past the Gap Map Method (GMM) is a very efficient approach for analysis of tunable^{9,10} and composite 1D PC^{11,12} as well as for PC structures with omnidirectional bands and defects^{13,14}. Thus, in the present paper the GMs of two-component and three-component PCs are presented and the influence of the t -layer on the transformation of SBs regions is demonstrated. Apart of this, the concept of PCs optical contrast alteration caused by the introduction of an additional regular t -layer is discussed and additional features in optical characteristics for this type of PC are demonstrated.

2. MODEL OF MULTI-COMPONENT PHOTONIC CRYSTAL STRUCTURE AND CALCULATION METHOD

2.1 Design of regular structure in three-component 1D Photonic Crystal.

The micro-structured Si with linear grooves¹⁵ is considered as the model for the 1D PC structure (Fig.1a). We use the refractive index of Si for high-refractive H component in IR range as $N_{Si}=N_H=3.42$. For the groove area, the refractive index of low-refractive L component is considered as $N_{air}=N_L=1$. In this case, the refractive index contrast is 3.42/1 and the consequent PC can be consider as a high-contrast PC. Therefore only a small number of periods m is needed to obtain a PBG with a reflectance of more than 0.999. Let us consider the minimal number of periods as $m=6$ and the maximum m number as $m=50$. The latter number results in PBGs with the same properties as those obtained from the Band Diagram (BD) method¹⁶. In this paper we are going to consider PC with different contrasts, namely 3.42/1.5, 3.42/2.21, 2.21/1 and 1.5/1. We are looking for the common tendencies in PBGs caused by insertion of an additional regular layer with different refractive indices N_i . During selection of N_i values we are going to pay particular attention to two very common cases in practical applications i.e. when N_i is varied between 3.42 and 1. In particular, in the case of $N_i=1.5$ we are dealing with an interlayer such as, for example, SiO₂ which can be deposited on Si walls with tunable thickness⁶, while value $N_i=2.21$ we can use to take into account the roughness of Si walls. In the latter case the optical characteristics of the roughness layer, N_i are equivalent to the effective homogeneous layer constructed from the combined parts of N_{Si} and N_{air} . This assumption holds if the parameters of roughness (rout-mean-square height and autocorrelation length) are much smaller than the wavelength of the incident light. The value of $N_i=2.21$ is obtained as the average value of the refractive indices of Si, N_{Si} and air, N_{air} . We also presume that the thickness of such an effective layer can be realized in a wide range of D_i values.

Optical properties of 1D PC are normally described, using BD method, in order to reveal the frequency ranges where the light propagation is absolutely prohibited for any polarization and for any direction of the wave vector. The calculations are normally performed for the PC with selected filling fraction $f_{Si}=D_H/A$, where A is the lattice constant of the periodical structure, and as the number of periods, m tends to infinity. The calculation of the reflectance spectra of 1D PCs with a certain number of lattice periods, m , can be performed using the Transfer-Matrix Method (TMM)¹⁷. The use of the latter method is attractive due to the ease of introducing any number of additional layers in any place of the TMM's equation

(see the next section). Obviously the reflectance spectra obtained for different filling fractions f can reveal certain changes.

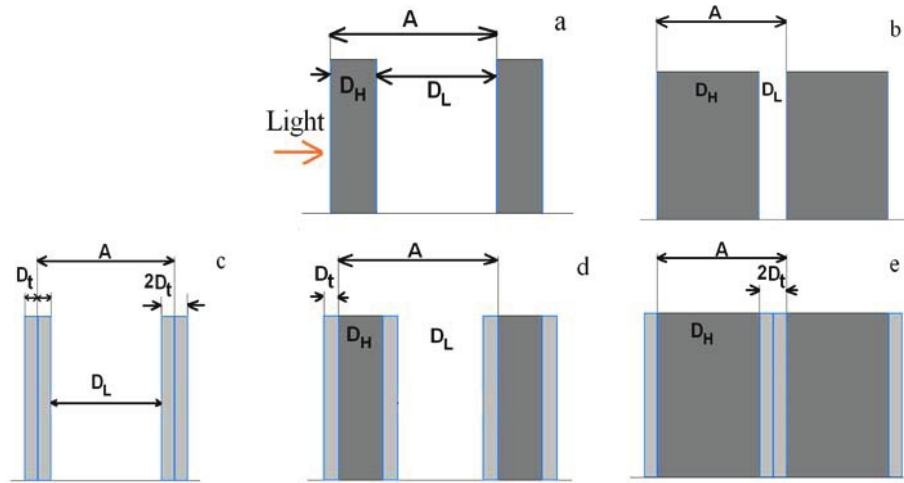


Fig.1. Schematic of two-component 1D PC (a,b,c,e) and three-component 1D PC (d) with fixed value of lattice constant A and an additional t -layer. The thicknesses of H , L and t -layer are D_H , D_L , D_t , accordingly. The filling fraction of Si, f is equal to $f_{Si}=0.26$ for the cases a) and d) and to 0.74 for b) and e).

in SBs as was shown in Ref.⁵. However, we believe that the best analysis of optical properties of multi-component PCs in general can only be obtained from a combination of TMM and gap map (GM) approaches⁹⁻¹³. This combination enables us to examine the optical properties of PC in general, using the possibility of selection of any number of periods, different filling fractions, introduction of any number of t -layers and then drawing all these dependences on one graph. Then the more detailed examination of the reflectance (transmission) spectra can be performed for some particular photonic structure.

2.2 Gap Map presentation for three-component Photonic Crystal.

We consider here normal incidence of light from the output media with $N=1$ on the front side of a PC structure (Fig.1a). First, let us calculate the reflectance spectra for 1D PC for a range of filling fractions from 0.01 to 0.99. Two 1D PC structures with the same lattice constant A and different filling fractions $f_{Si}=0.26$ and 0.74 are shown as an example on the Fig. 1a and Fig 1b, respectively. For each of the calculated reflectance spectra the region of NF, where the reflectance was greater than 0.999, was recorded on the graph. Thus obtained PBG ranges were then plotted, together with all the other filling fractions, to give a graph that is called a gap map. The end result is displayed in Fig. 2 for the optical contrast 3.42/1 and number of periods $m=50$. The graph gives a number of PBGs where the reflectance is greater than 0.999. For GM and spectra calculations all the optical characteristics are presented in normalized frequency units and therefore can be applied to a wide range of structure sizes including micro- and nano-structures.

In order to create GM we need to generate the filling fraction $f_{Si}=D_H/A$ ranging from 0 to 1. We assume that the lattice constant A and t -layer thickness D_t do not change since the t -layers with refractive index N_t were introduced on both sides of Si wall H in our PC structure (Fig. 1d). The generation of D_H for both the two-component and the three-component PCs occurs with the same values. According to this, the D_L varies due to decreasing of L -layer after introduction of t -layer with thickness D_t on both sides of Si walls D_H (Fig.1d). In this approach we use D_H for both the two-component PC and for three-component PC and thus we can compare two different PC structures using one f_{Si} scale.

Schematically, the Transfer Matrix S_2 for two-component PC structure can be presented in the following form¹⁷:

$$S_2=(M_H \cdot M_L)^m M_H \quad (1)$$

while for three-component PC matrix S_3 it can be written as:

$$S_3=(M_t M_H M_L \cdot M_L)^m M_t M_H M_t \quad (2)$$

where M_H , M_L and M_t are matrices of H , L and t layers accordingly.

In accordance with Fig. 1d, D_L decreases after the introduction of D_t . As a result during GM drawing not all the filling fractions values f_{Si} from 0.01 to 0.99 can be realized in such a PC. The larger the value D_t , the lower the maximum value of filling fraction f_{Si} that can be realized in the three-component PC. As a numerical example let us consider $A=3 \mu\text{m}$. This leads to change in Si wall thickness $D_H=A \times f_{Si}$ from 0.03 to $2.97 \mu\text{m}$. The t -layer thickness was taken, for example, as $D_t=0.4 \mu\text{m}$ and it corresponds to the parameter $D_t=0.13A$. In Table 1 the maximum values of filling fractions f_{Si} obtained for different values of t -layer D_t are presented.

Table 1. The maximum value of filling fraction $\text{Lim}f_{Si}$ for different values of t -layer thicknesses D_t , needed for GM calculations of three-component PC with $A=3 \mu\text{m}$.

$D_t, \mu\text{m}$	0.1	0.2	0.3	0.4	0.6	0.8	1.0	1.2	1.4
D_t/A	0.03	0.07	0.10	0.13	0.20	0.27	0.33	0.40	0.47
$\text{Lim}f_{Si}$	0.94	0.86	0.80	0.74	0.60	0.46	0.34	0.20	0.06

As can be seen from Table 1, the GM for the three-component PC can be calculated only up to the definite maximum value of filling fraction f_{Si} depending on the parameter D_t . The generation of D_H doesn't occur for all filling fractions over that maximum value, as if the real PC doesn't exist for these particular values of f .

3. ANALYSIS OF STOP BANDS AND REFLECTANCE SPECTRA FOR TWO-COMPONENT AND THREE-COMPONENT PHOTONIC CRYSTALS

3.1 Influence of t -layer thickness on Gap Map formation

Let us calculate the GM for the PC with number of periods $m=50$ (which is practically similar to the PC with an infinite number of periods) and with $D_t=0.13A$. As can be seen in the Fig.2, the $\text{Lim}f_{Si}$ restricts the formation of PBG according to the data presented in Table 1. Hence, the GM was drawn for SBs calculated for the range of filling fractions f_{Si} from 0 to 0.74.

It can be also seen from Fig.2, that the introduction of t -layer with $D_t=0.13A$ and $N_t=1.5$ results in i) a decrease in every SB and ii) in the red shift of SBs. In the limiting case, as the t -layer thickness D_t increases up to the maximum value, the L component tends to disappear and be totally replaced by the t -layer (Fig.1e). In this case we obtain the two-component PC again but with a different optical contrast, namely $3.42/1.5$. Indeed the cutoff line at $f_{Si}=0.74$ intersects two SBs areas for the first, three-component PC ($D_t=0.13A$) and, the second, two-component PC but with a different contrast $N=3.42/1.5$ (Fig.2a). In Fig. 2b the first SBs were considered for PC structures with different t -layer thicknesses. The red shift of the SB's blue edge as D_t increases can be also seen from this figure. A similar behavior was observed earlier for L -component in two-component PC as N_L increased^{10,11}.

The dependence of SB width versus filling fraction f_{Si} and thickness D_t is presented in Fig.3. The decrease in SB width and the shift of the maxima to the region of high f_{Si} values with increase of the t -layer thickness can be seen from the figure. This is a typical behavior of SBs with a decrease of the optical contrast. Thus, the introduction of t -layer causes a similar effect as the substitution of N_L . However, in our case the range of possible f_{Si} values decreases significantly, for example at $D_t=0.33A$ the values of f_{Si} range from 0 to 0.34 (Fig.2b). It is worthwhile to mention that the widest SBs are observed for this particular range of f_{Si} . We can conclude that the employment of three-component PC can be used as an alternative for alteration of the optical contrast of PC and, therefore, for tuning the position and the width of SBs in reflectance/transmission spectra.

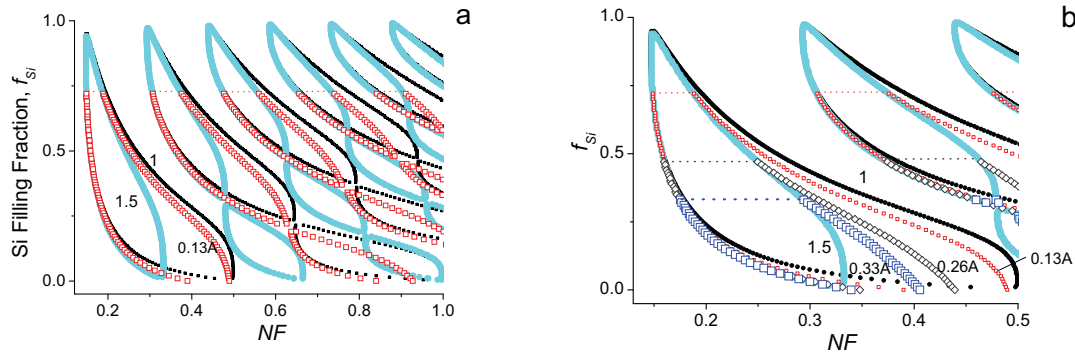


Fig.2. Stop Bands red shift caused by introduction of t -layer with refractive index $N_t=1.5$ and thicknesses D_t (denoted by numbers on curves) into the ordinary, two-component 1D PC with contrast $N=3.42/1$ (number 1, black solid circles) and number of periods $m=50$. For comparison, the SBs of two-component PC with contrast $N=3.42/1.5$ are also shown (number 2, gray solid circles): a) Stop Bands for the NF range from 0 to 1, b) the first and high order Stop Bands with cutoff lines at $f_{Si}=0.74$ for $D_t=0.13A$, $f_{Si}=0.48$ for $D_t=0.26A$ and $f_{Si}=0.34$ for $D_t=0.33A$.

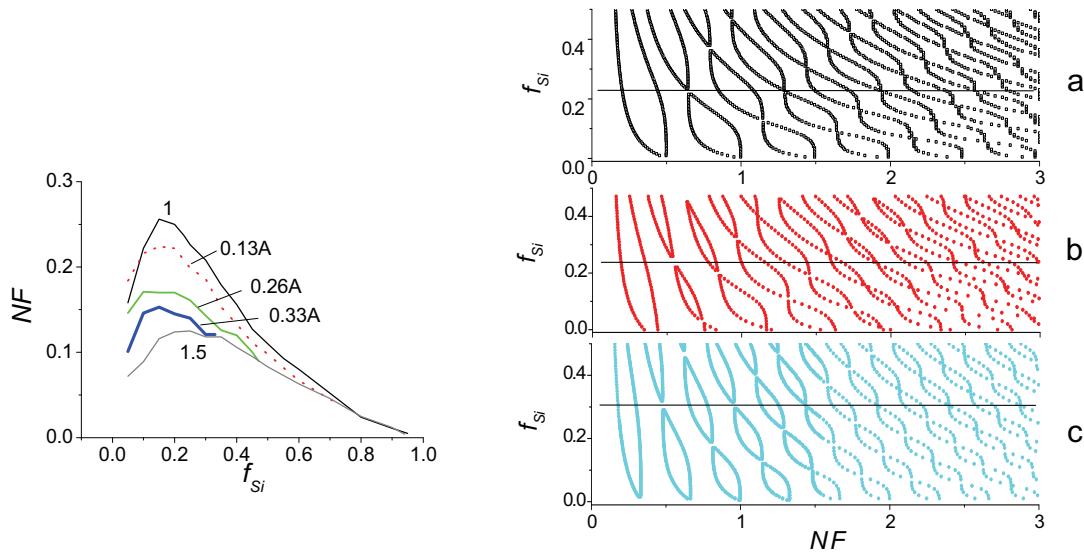


Fig.3. The first SBs width vs. f_{Si} and t -layer thickness at $N_t=1.5$ (from Fig.2b).

Fig.4. The influence of t -layer with $D_t=0.26A$ and $N_t=1.5$ on the size of higher order SBs in multi-component PC (b). This compares to ordinary PC with (a) high optical contrast 3.42/1 and (c) middle contrast 3.42/1.5 in a wide range of NF .

Let us analyze the GM for the multi-component PC in a wide range of NF from 0 to 3 (Fig.4 b) and compare this with GM for the two-component PCs (Figs. 4a and 4c), but with different contrasts N . For example, we can use the three-component PC with thickness of t -layer $D_t=0.26A$ correspondent to the cutoff line at $f_{Si}=0.48$. As can be seen from the Figs.4a and 4c, the size of SBs for ordinary PCs obviously decreases with their order, while for the three-component PCs these changes are not so regular. For the ordinary PC the edge points of SBs correspondent to the constructive interference are aligned along one line (for a certain value of f_{Si}) with increase of NF , while no such behavior was revealed for the three-component PC (see Figs. 4 a, b, c). Therefore, even without clearly understanding the reasons that cause such a phenomenon, the Gap Map drawn for three-component PC enables us to predict the appearance/disappearance and the width of SBs as a function of f_{Si} and to use the higher order SBs as it was suggested earlier⁹.

It is important to analyze how the quality of the reflectance bands within SBs are changed under the influence of different perturbations, since these can cause the reduction of the absolute values of R (down to 0.9 or even lower values), the band shape changes and other types of band degradation. An additional t -layer with optical thickness equal to $N_t \times D_t$ contributes to the total interference of the reflected wave but doesn't destroy the R value in SBs, i.e. the reflectance is still more than 0.999. However, this is true only under a rough estimation. As can be seen from the Fig.5, for the first SBs with filling fraction $f_{Si}=0.23$ the value of $T=1 \times 10^{-15}$ is very small and this doesn't change with D_t . Therefore, we can conclude that the introduction of the additional t -layer doesn't affect the properties of the first SBs and hence should not be consider as a degradation factor in this case.

3.2 The influence of t -layer refractive index N_t on the formation of stop-bands.

Let us consider how the SB changes if the refractive index of t -layer N_t is varied from 1.5 to 2.21. In order to check this, let us select $D_t=0.13A$ and perform the calculation of SBs up to the definite value of the f_{Si} from 0 to 0.74. The red shift of the SB's blue edge at $N_t=2.21$ (Fig. 6) is larger, than for the PC at $N_t=1.5$ (Fig. 2) for the same thickness of t -layer. This result is quite predictable, because the optical thickness of t -layer ($N_t \times D_t$) increases with N_t and, as was already mentioned, the increase of the optical thickness reduces the optical contrast. The SB's shape changes for the t -layer at $N_t=2.21$. Let us look on the lower part of SB's for the multi-component PC at $f_{Si}=0$ shown in Figs. 6a and 6b. Contrary to the ordinary (two-component) PC, the short-wavelength and long-wavelength edges of SBs do not coincide. If the Si wall is not presented in the PC structure, then the periodical structure is now formed from the t -layers and L -component. Thus, the total t -layer thickness is equal to $2 \times D_t=0.26A$ (Fig.1c). Every double t -layer is separated from the next one by a definite air gap with $N_L=1$. These layers create the periodical structure with the lattice constant $A=3 \mu m$ and can possess the PBGs correspondent to the optical contrast of 2.21/1 value. Now, we can draw the GM for this contrast for the number of period $m=50$ and we can see the first SB presented in Fig.7.

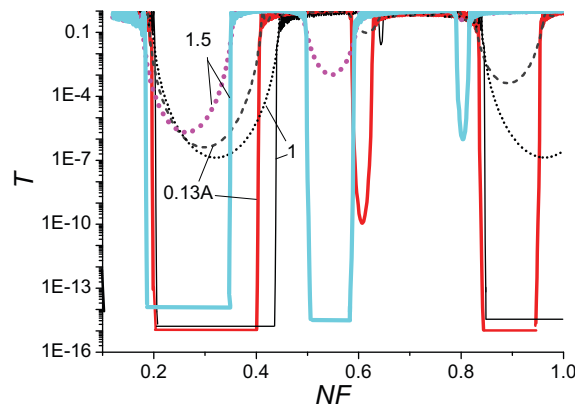


Fig.5. The transmission spectra of the first and second SBs for the PCs with optical contrasts 3.42/1 (curves 1) and 3.42/1.5 (curves 1.5) and for the three-component PC with $m=50$ (solid line) and $m=6$ (dotted line) with additional layer of $D_t=0.13A$ (dashed line).

Let us draw a horizontal line at $f_i=0.26$ as shown in Fig. 7. By doing this we can obtain the edges of the first SB from 0.29 to 0.47 NF . These are exactly the values of NF that we can see in Fig.6 for $f_{Si}=0$. By analogy, the same can be done for the above considered additional t -layer with $N_t=1.5$. We need first to calculate the GM for two-component PC with contrast 1.5/1 for the definite t -layer thickness of $D_t=0.13A$ and to determine the value of f_{2t} , that gives us the NF range for the first SB. The NF range, obtained earlier, corresponds to the NF range for $f_{Si}=0$ in Fig.2. Therefore, the NF range appearance for $f_{Si}=0$ for the considered three-component PC model are explained. This can occur when two additional t -layers with $N_t=1.5$ (or 2.21) are hypothetically joined in one layer, thus forming the ordinary (two-component) PC with correspondent optical contrasts.

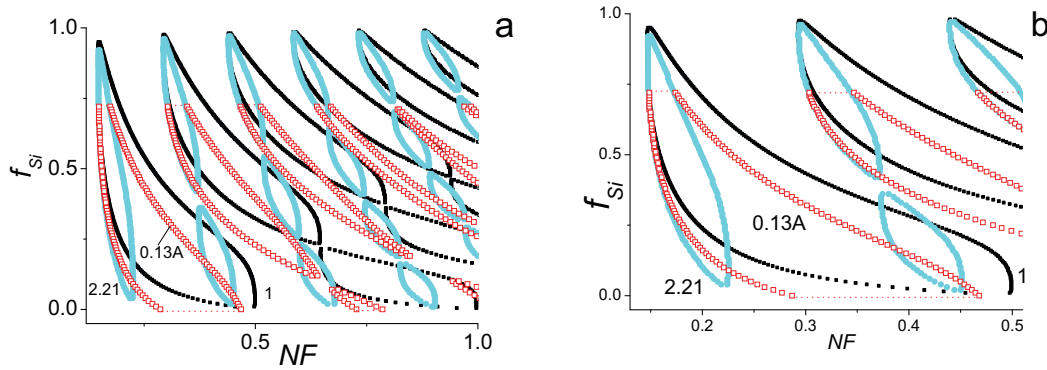


Fig.6. The gap map of SBs for the ordinary (two-component) PC with contrast $N=3.42/1$ (number 1, black solid circles) and number of periods $m=50$ and for the three-component PC, obtained by introduction of t -layer with refractive index $N_t=2.21$ and thickness $D_t=0.13A$ (shown by number at the edge of the band) for the range of NF from 0 to 1. For comparison, the SBs regions of the ordinary (two-component) PC with contrast $N=3.42/2.21$ (shown by number 2.21, thick line). a) SBs for the range of NF from 0 to 1 b) The range of the first SB with cutoff line at $f_{Si}=0.74$ for $D_t=0.13A$.

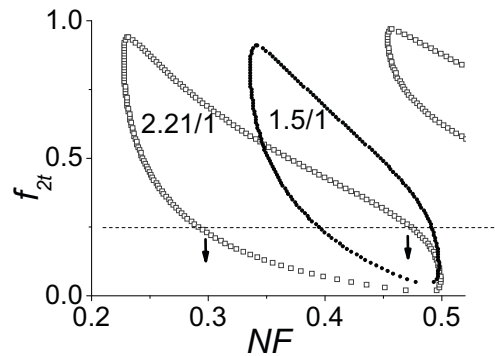


Fig.7. The range of the first SBs for the ordinary (two-component) PCs with contrast 2.21/1 and 1.5/1. The dotted line demonstrates the regions of NF for the value of filling fraction $f_{2t}=0.26A$ (see Fig. 1c) for two PCs.

3.3 Influence of the number of periods on the formation of stop-bands in three-component PC.

The next step is to determine how SBs change for the smaller number of periods, for example for $m=6$. Let us to analyze some changes in the first SBs depending on the thickness of the additional t -layer (Fig. 8).

In comparison with 50-period ordinary PC the 6-period PC has a narrower first SB. This effect is more dramatic as N_t increases up to 2.21 due to a significant shift between the first stop-bands for the two-component PCs with low-contrast (3.42/2.21) and high-contrast (3.42/1) (Fig.8b). Thus the introduction of a t -layer with $N_t=2.21$ leads to a red-shift of SB's blue edges and to a decrease of the PC contrast which is more significant than that seen for $N_t=1.5$

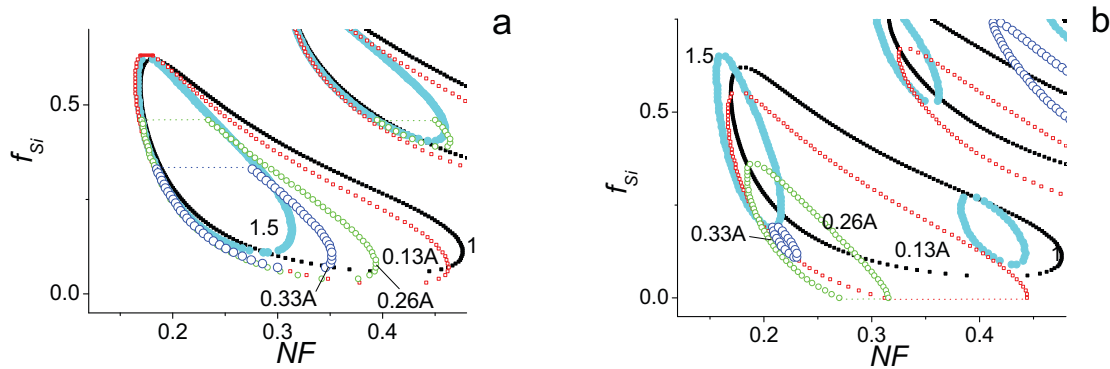


Fig.8. The range of the first SB for the ordinary 1D PCs with contrasts $N=3.42/1$ (denoted as 1) and $3/42/1.5$ (denoted as 1.5) and for three-component PC with $D_t = 0.13A$, $0.26A$ and $0.33A$ at number of periods $m=6$ for the values of t -layer $N_t=1.5$ (a) and $N_t=2.21$ (b)

Let us examine now what happens to SBs for the ordinary PC with $m=50$ using the GM presentation after the introduction of t -layer with $D_t=0.13A$ and $N_t=1.5$ for wide range of NF (Fig.9). We can see that the obtained SBs for three-component PC with $m=50$ decrease. This effect has already been explained above as the result of the decrease in PC contrast. Then, with the decrease of m to a value of 6 only small stop-bands disappear (Fig.9 and Fig. 10 a). This is due to the fact that the value of R for these SBs becomes smaller than 0.999 (Fig 10 c). The vanishing of SBs, caused by introduction of the additional layer, was also mentioned in Ref.⁸. As can be also seen from Fig. 9, the most stable stop-bands are the first ones and the nearest secondary bands. At the same time the maximum transmission value T has increased by five orders of magnitude in the logarithmic scale in comparison to the ones at $m=50$ with consequent dramatic change in the shape of the stop-bands in the T -spectrum (Fig. 5). However the maximum transmission value is still not larger than 10^{-5} . The gap map transfers to a slightly different form (Fig.10 a,d) with an increase of N_t to 2.21, i.e. with a decrease in the optical contrast.

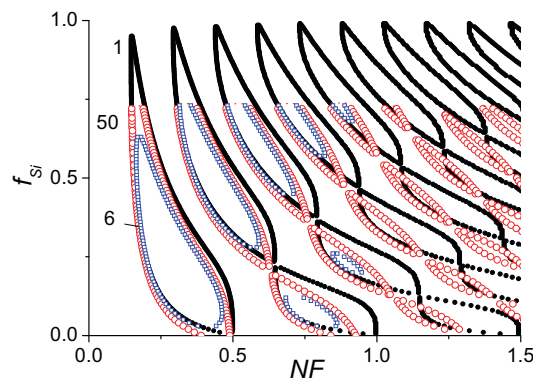


Fig.9. SBs maps for ordinary PC with contrast 3.42/1, $m=50$ (1), for three-component PC with $D_t=0.13A$, $N_t=1.5$ and $m=50$ (50) and $m=6$ (6).

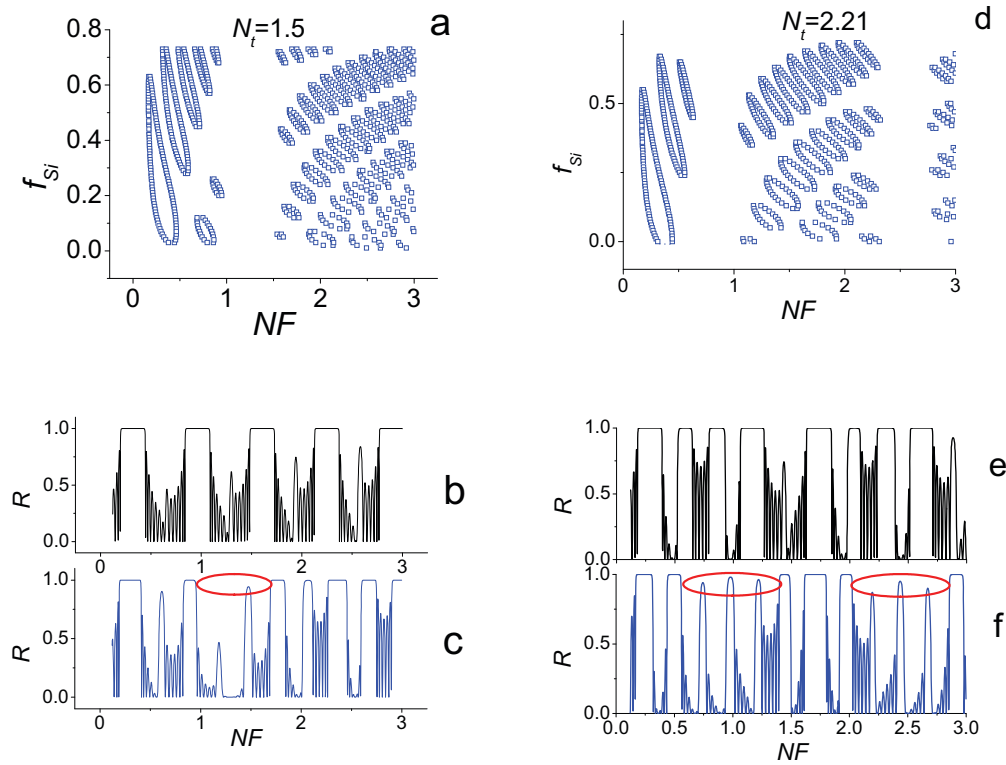


Fig. 10. (a,d) The GMs of SBs and the reflectance spectra R for three-component PC with $m=6$, $D_t=0.13A$. The suppression of high order SBs for $N_t=1.5$ (c) и $N_t=2.21$ (f) is shown. For comparison, the reflectance spectra R for ordinary (two-component) PC with $f_{si}=0.23$ (b) and $f_{si}=0.3$ (e) are also presented.

Two ranges of NF , where the SBs disappeared, are seen from the GM shown in Fig.10d. This can be confirmed by the reflectance spectra shown in Fig.10f. Thus, the introduction of the additional layer with definite optical thickness at certain conditions prevents the formation of constructive interference (which is the composition of re-reflected wave amplitudes) and leads to the shift and vanishing of the maxima in spectra R and in GM. To answer the question, why the NF range is constant for one definite optical thickness of the additional layer and doesn't depend on f_{si} , while at the same time the optical thickness on its own depends on f_{si} , further investigations are necessary.

4. CONCLUSION

In this paper, the three-component PC structure was presented using the model of ordinary (two-component) PC structure with the insertion of an additional layer on both sides of the high-refractive (H) component. The investigation of this three-component PC was made using the gap map approach at the normal incidence of light. The ordinary (two-component) PCs were also considered for comparison. During stop-bands map calculations for three-component PC the limited value of filling fraction for H layer, caused by the additional t -layer, was taken into account. As a result of an additional t -layer introduction into ordinary (two-component) PC with optical contrast $N=3.42/1$, the SB's red-shift was detected. The blue edge of the first SB for the three-component PC has been found in the middle between the SB's for

two ordinary (two-component) PCs with different contrasts N . It has been demonstrated that it is possible to change PC contrast not only by using different fillers, but also by the insertion of an additional layer enabling the fine tuning of the position of SB's edge. The influence of the number of period, m and the optical contrast, N_i on SBs properties was investigated. It was found, that PBG vanishes for the regions of higher order stop-bands in the gap map with small number of periods. This effect becomes stronger with an increase in N_i from 1.5 to 2.21.

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