One-dimensional photonic crystals with highly Bi-substituted iron garnet defect in reflection polar geometry

T V Mikhailova, V N Berzhansky, A V Karavainikov, A N Shaposhnikov, A R Prokopov and S D Lyashko
V.I. Vernadsky Crimean Federal University, 4 Vernadskogo Prospekt, Simferopol, 295007, Russia

Abstract. It is represented the results of modelling of magnetooptical properties in reflection polar geometry of one-dimensional photonic crystal, in which highly Bi-substituted iron garnet defect of composition Bi\textsubscript{1.0}Y\textsubscript{0.5}Gd\textsubscript{1.5}Fe\textsubscript{4.2}Al\textsubscript{0.8}O\textsubscript{12} / Bi\textsubscript{2}Fe\textsubscript{2}O\textsubscript{12} is located between the dielectric Bragg mirrors (SiO\textsubscript{2} / TiO\textsubscript{2})\textsuperscript{m} (were \textit{m} is number of layer pairs) and buffer SiO\textsubscript{2} and gold top layers of different thicknesses is placed on structure. The modification of spectral line-shapes of microcavity and Tamm plasmon-polariton modes depending on \textit{m} is found.

1. Introduction
One-dimensional photonic crystals (1D-PCs) [1] are artificial optical-order periodic structures, that can affect the propagation of light and actively used for micro- and nano- optoelectronic devices, displays, information transmitting devices, storage, magnetic holography and sensors. The functionality of such devices may be based on the magnetooptical (MO) effects, Faraday and polar Kerr effects, that occur in included in 1D-PC structure magnetoactive (MA) defect. The transparent Bi-substituted iron garnet (Bi:IG) films may be taken as a defect. Enhancing of MO effects defect due to the phenomena of interference and diffraction in 1D-PC reaches record values of 20 times at visible [2] and 100 times at near infrared [3] ranges of wavelengths. Recently research of MO effects in 1D-PCs, in which the simultaneous excitation of several resonance modes (microcavity or defect, Tamm plasmon-polariton, surface plasmon-polariton, exciton) exist, also became relevant.

This work predominantly focuses on the investigation of microcavity and Tamm plasmon-polariton modes in modelled polar Kerr rotation (KR) spectra of 1D-PCs [TiO\textsubscript{2}/SiO\textsubscript{2}]\textsuperscript{m} / Bi\textsubscript{1.0}Y\textsubscript{0.5}Gd\textsubscript{1.5}Fe\textsubscript{4.2}Al\textsubscript{0.8}O\textsubscript{12} / Bi\textsubscript{2}Fe\textsubscript{2}O\textsubscript{12} / [SiO\textsubscript{2}/TiO\textsubscript{2}]\textsuperscript{m} with addition of buffer SiO\textsubscript{2} and gold top layers of different thicknesses. The model is based on the fitting parameters of the synthesized 1D-PCs without buffer SiO\textsubscript{2} and gold top layers. Optimality of multiresonance 1D-PCs for application depends on the Bi:IG layers absorption, that are most strongly manifested in the visible range of wavelengths and that contribution was not previously observed in the polar Kerr effect modelling or experimental study [4].

2. Synthesis of 1D-PCs with highly Bi:IG defect. Experimental reflectance and polar Kerr rotation spectra
As was found previously in our investigations to create nanostructures of 1D-PCs with highly Bi:IG defect and high optical quality necessary to satisfy the optimal synthesis conditions. Thus, the double MA defect of composition Bi\textsubscript{1.0}Y\textsubscript{0.5}Gd\textsubscript{1.5}Fe\textsubscript{4.2}Al\textsubscript{0.8}O\textsubscript{12} / Bi\textsubscript{2}Fe\textsubscript{2}O\textsubscript{12} (the buffer layer Bi\textsubscript{1.0}Y\textsubscript{0.5}Gd\textsubscript{1.5}Fe\textsubscript{4.2}Al\textsubscript{0.8}O\textsubscript{12} hereinafter is M1 and the main layer Bi\textsubscript{2}Fe\textsubscript{2}O\textsubscript{12} hereinafter is M2) in
considered 1D-PCs caused by the technological difficulties of synthesis of garnet films with a high Bi content on SiO$_2$ layers. Bi:IG layers were fabricated by reactive ion beam sputtering of corresponding ceramic targets in argon-oxygen mixture on "cold" fused quartz substrate KU-1 and crystallized in the annealing process at the air. High (up to 80%) oxygen content in the sputtering gas mixture and low heating rates during annealing crystallization used to achieve low surface roughness of the Bi:IG layers. M1 and M2 layers were formed and crystallized separately at optimal annealing temperature of 680 °C. The first layer M1 was deposited on SiO$_2$ and after its crystallization the layer M2 was deposited and crystallized. The thickness of MA layers was controlled by the sputtering rates and the deposition times. Necessary MO and the crystalline quality of the double layer is achieved at the minimum optimal thickness of the buffer layer, which approximately corresponds to the optical thickness $\lambda_0/4$, where $\lambda_0$ is the wavelength of photonic band gap (PBG) center. TiO$_2$ and SiO$_2$ layers were fabricated by electron beam evaporation with an optical thickness control by monitor in-situ. To minimize the size and influence of transition layer "substrate – structure" ion-beam treatment of the substrates (low-energy plasma of Ar$^+$, ion current density 2.5 mA cm$^{-2}$) was applied.

The experimental and theoretical spectra of polar KR and reflectance of synthesized 1D-PCs with MA defect of (2.5-$\lambda_0$/2)-optical thickness and repetition number of layer pairs $m = 4$ and $m = 7$ are shown in Figure 1 (data taken from [2]). MA defect of thickness $h_M = 317$ nm includes a buffer layer M1 of thickness $h_{M1} = 68$ nm. PBG center is $\lambda_0 = 685$ nm. The thicknesses of SiO$_2$ and TiO$_2$ layers are $h_{SiO_2} = 116$ nm and $h_{TiO_2} = 75$ nm, respectively. For these structures the maximum Faraday rotation –13.6 and –20.6 deg and MO quality factor 15.1 and 8.0 deg have been achieved for resonance at 625 nm for $m = 4$ and $m = 7$, respectively.

![Figure 1](image)

**Figure 1.** Spectra of polar Kerr rotation $\theta_K$ (a, b) and reflectance $R$ (c, d) of synthesized 1D-PCs with highly Bi:IG defect of (2.5-$\lambda_0$/2)-optical thickness and different number $m$ [2].

As will be shown in subsection 3.1, the number of resonance peaks (one or two) in PBG corresponding to first I, second II or third III microcavity modes (with resonance conditions ($\lambda_0$/2), ($\lambda_0$) or (3-$\lambda_0$/2), respectively) and their spectral position depends on the thickness of MA defect (or its optical thickness $h_0$). In Figure 1 the spectra include II and III microcavity modes at 760 and 625 nm, accordingly. The features of polar KR spectra of considered 1D-PCs without gold top layer are a large positive peak and two minor negative asymmetric peaks in the vicinity of the resonance wavelengths.
In contrast to the Faraday rotation values the maximum polar KR observed at 625 nm for the structures with \( m = 4 \) (\( \Theta_k = -8.9 \) deg), but not with \( m = 7 \) (\( \Theta_k = -1.7 \) deg).

3. Polar Kerr rotation spectra modelling

The light propagation in 1D-PCs were modelling by computational solution of Maxwell's equation

\[
\nabla \times \mathbf{E}(r,t) = i\omega\mu_0 \mathbf{H}(r,t), \quad \nabla \times \mathbf{H}(r,t) = -i\omega\varepsilon_0 \mathbf{E}(r,t)
\]

by conventional 4×4 transfer matrix method [5]. Here \( \mathbf{E}(r,t) \) and \( \mathbf{H}(r,t) \) are magnetic and electric fields vectors of light wave respectively, \( \mathbf{r} \) is radius-vector, \( t \) is time, \( \mu_0 \) and \( \varepsilon_0 \) are vacuum permeability and permittivity respectively, \( \hat{\varepsilon} \) is the permittivity tensor of corresponding layer. For optical frequencies \( \mu = 1 \), General view of \( \hat{\varepsilon} \) is

\[
\hat{\varepsilon} = \begin{pmatrix}
\varepsilon_{xx} & -i\varepsilon_{xy} & 0 \\
 i\varepsilon_{yx} & \varepsilon_{yy} & 0 \\
 0 & 0 & \varepsilon_{zz}
\end{pmatrix}.
\]

Components \( \varepsilon_{xx} \) and \( \varepsilon_{yy} \) for MA layers are complex, \( \varepsilon_{xx} = \varepsilon'_{xx} + i\varepsilon''_{xx}, \varepsilon_{yy} = \varepsilon'_{yy} + i\varepsilon''_{yy} \). The value of \( \varepsilon''_{xx} \) is very close to \( \varepsilon_{xx} \) below Curie temperature \( T_C \) and is equal to \( \varepsilon_{xx} \) above \( T_C \). Component \( \varepsilon_{xx} \) determines by refractive index \( n \) and extinction coefficient \( k: \varepsilon_{xx} = (n^2 - k^2) + i \cdot 2 \cdot n \cdot k \). Component \( \varepsilon_{yy} \) relates to Faraday rotation \( \Theta_F \), magnetic circular dichroism \( \Delta \alpha \), refractive index \( n \), extinction coefficient \( k \) of film and wavelength of incident light \( \lambda \) as

\[
\varepsilon'^{xy} = -\left(\frac{\lambda}{\pi}\right) \left( n \cdot \Theta_F + \frac{k \cdot \Delta \alpha}{4} \right), \varepsilon'*_{yy} = -\left(\frac{\lambda}{\pi}\right) \left( \Theta_F \cdot k - \frac{n \cdot \Delta \alpha}{4} \right)
\]

For nonmagnetic layers of BM \( \varepsilon_{yy} = 0 \) and \( \varepsilon''_{xx} = \varepsilon_{xx} \). It is considered that TM polarized light falls to the structure. The fused quartz substrate KU-1 and the spectral dependence of permittivity tensor components of layers taken into account. Components of permittivity tensor of 1D-PC layers is defined using the experimental data of single films and synthesized 1D-PCs and presented in Table 1. These values are used for shown in Figure 1 calculations and below.

### Table 1. Permittivity tensor components for layers of model 1D-PCs

| Wavelength (\( \lambda \)) (nm) | M1 \( \varepsilon_{xx}^1, \varepsilon_{xy}^1 \) | M2 \( \varepsilon_{xx}^2, \varepsilon_{xy}^2 \) | SiO\(_2\) and KU-1 \( \varepsilon_{SiO_2}, \varepsilon_{KU-1} \) | TiO\(_2\) \( \varepsilon_{TiO_2} \) | Au \( \varepsilon_{Au} \) |
|-----------------------------|--------------------------------|--------------------------------|-----------------------------|-----------------------------|-----------------------------|
| 600                        | \( 7.039 + 0.121 \cdot i \), \( -0.014 + 2.656 \cdot 10^{-3} \cdot i \) | \( 8.35 + 0.177 \cdot i \), \( -0.072 + 0.019 \cdot i \) | 2.125                       | 5.409                       | \(-9.34 + 1.47 \cdot i \) |
| 650                        | \( 6.591 + 0.066 \cdot i \), \( -9.187 \cdot 10^{-3} + 2.702 \cdot 10^{-3} \cdot i \) | \( 7.863 + 0.063 \cdot i \), \( -0.037 + 0.01 \cdot i \) | 2.12                        | 5.282                       | \(-12.864 + 1.198 \cdot i \) |
| 700                        | \( 6.277 + 0.038 \cdot i \), \( -7.37 \cdot 10^{-3} + 2.813 \cdot 10^{-3} \cdot i \) | \( 7.518 + 0.044 \cdot i \), \( -0.024 + 7.801 \cdot 10^{-3} \cdot i \) | 2.117                       | 5.182                       | \(-16.519 + 1.113 \cdot i \) |
| 750                        | \( 6.06 + 0.021 \cdot i \), \( -6.619 \cdot 10^{-3} + 2.95 \cdot 10^{-3} \cdot i \) | \( 7.279 + 0.041 \cdot i \), \( -0.018 + 7.886 \cdot 10^{-3} \cdot i \) | 2.114                       | 5.102                       | \(-20.22 + 1.122 \cdot i \) |

Thus, the following structure is taken as a model

\[ \text{KU-1} / [\text{TiO}_2/\text{SiO}_2]^m / \text{M1} / \text{M2} / [\text{SiO}_2/\text{TiO}_2]^m / \text{SiO}_2 / \text{Au} \]
with thicknesses of M1 layer $h_{M1} = 68$ nm, SiO$_2$ and TiO$_2$ layers of 1D-PC $h_{SiO_2} = 116$ nm and $h_{TiO_2} = 75$ nm, respectively. M2 $h_{M2}$, top gold $h_{Au}$ and top buffer SiO$_2$ $h_{SiO_2}$ layers thicknesses and repetition number of layer pairs $m$ are varied depending on the calculations purpose.

3.1. 1D-PC with highly Bi:IG defect of different optical thickness and without top SiO$_2$ and gold layers

Figure 2 shows the spectral displacement of resonance peaks corresponding to I, II and III microcavity modes occurring with increasing of optical thickness of MA defect. The thickness of MA defect is augmented by change of M2 layer thickness $h_{M2}$. For ($\lambda_0/2$), ($1.5\cdot\lambda_0/2$), ($2\cdot\lambda_0$) and ($3\cdot\lambda_0/2$)-structures the values of $h_{M2}$ are 64, 126, 193, 244 and 315 nm, respectively. The modification of KR peaks is absent. Dependence of polar KR on the number $m$ for I microcavity mode in Figure 3 (a) demonstrates the achievement of maximum KR for 1D-PC with optimum repetition number of layer pairs $m_{opt} = 4$, as the experiment show earlier (see section 2). It is caused the growing influence of significant absorption of highly Bi:IG during the amplification of the light localization inside the defect with increasing of number $m$. It is evident from the transmittance and reflectance shown here. The optimum value of $m_{opt}$ is different for each resonance modes and changes with the its shifting in PBG. Figure 3 (b) shows the polar Kerr rotation as a function of the number $m$ for I and II microcavity modes. KR can be increased by shifting of cavity mode from the PBG center to longer wavelengths with increasing of $m_{opt}$ (curves 2 and 3) or by a change of the microcavity mode at the BPG center wavelength with increasing of $h_{M2}$ and decreasing of $m_{opt}$ (curves 1 and 4).

![Figure 2. Polar Kerr rotation spectra of model 1D-PC with MA defect of ($\lambda_0/2$), ($1.5\cdot\lambda_0/2$), ($2\cdot\lambda_0$) and ($3\cdot\lambda_0/2$)-optical thickness (curves 1, 2, 3, 4 and 5, respectively). Repetition number of layer pairs is $m = 4$. The arrows indicate the displacement of microcavity modes. Curves is shifted up to 5 degrees relative to the previous curve on the scale of polar Kerr rotation.](image)

![Figure 3. (a) Reflectance $R$, transmittance $T$ and polar Kerr rotation $\Theta_K$ as a function of the number $m$ of model 1D-PC with MA defect of ($\lambda_0/2$)-optical thickness. (b) Polar Kerr rotation $\Theta_K$ as a function of the number $m$ for I microcavity mode of model 1D-PC with MA defect of ($\lambda_0/2$) and ($1.5\cdot\lambda_0/2$)-optical thickness (curves 1 and 2, respectively) and for II microcavity mode of model 1D-PC with MA defect of ($1.5\cdot\lambda_0/2$), ($2\cdot\lambda_0$) and ($2.5\cdot\lambda_0/2$)-optical thickness (curves 3, 4 and 5, respectively).](image)
3.2. 1D-PC with highly Bi:IG defect of (λ/2)-optical thickness and top gold layer and without top SiO₂ buffer layer

For the 1D-PC structure with the top gold layer the modification of line-shape of microcavity mode takes place. The Tamm plasmon-polariton mode is observed in the wavelength range from 740 to 850 nm and its behaviour is considered in subsection 3.3. The inversion of KR peak of microcavity mode occurs for 1D-PC with \( m = 4 \) at increasing of gold layer thickness \( h_{Au} \) from 0 to 200 nm, that is shown in Figure 4. For structures with \( m < 4 \) the line-shape and sign of microcavity mode are similar to the line-shape and sign of Faraday rotation peaks. For the structure with \( m > 4 \) the line-shape of KR peak is similar to that shown in Figures 1 and 2 for 1D-PC without the top gold layer. The spectral position of the resonance peak is strongly dependent on the number \( m \). The maximum KR is achieved at "inversion region" for \( m = 4 \) \( \Theta_{KR} = 17.7 \) deg and \( m = 5 \) \( \Theta_{KR} = 21.3 \) deg. So, for the structures with \( m = 5 \) the presence of a top gold layer increases the KR by 4 times at preservation the line-shape of the resonance peak. The inversion of KR peak is caused by the competition of "passing through" (absorbed) and "reflected by" MA layer contributions to the polarization rotation angle of 1D-PC.

![Figure 4. Spectra of polar Kerr rotation \( \Theta_{KR} \) of model 1D-PC with MA defect of (λ/2)-optical thickness for I microcavity mode as a function of the thickness \( h_{Au} \) for the number \( m = 4 \) (a) and as a function of the number \( m \) at unchanged thickness \( h_{Au} = 200 \) nm (b).](image)

3.3. 1D-PC with highly Bi:IG defect of (λ/2)-optical thickness and top buffer SiO₂ and gold layers

Spectral position and line-shape of Tamm plasmon-polariton mode depend on the introduction of the buffer layer in structure before top gold layer. To reduce the absorption of used materials as the buffer layer the SiO₂ layer of thickness \( h_{SiO₂} \) has been selected, but the MA layer can also be applied. Figure 5 shows the modification of KR spectra of considered 1D-PC with unchanged top gold layer thickness \( h_{Au} = 200 \) nm versus number \( m \) and the thickness \( h_{SiO₂} \), which is varied from 174 to 232 nm.

When a buffer layer is absent, the spectral position of Tamm plasmon-polariton mode corresponds to PBG long-wave edge, similarly to that shown in Figure 5 (e) and (f). When \( m \) changes its spectral position and line-shape also change. S-shape peak is observed for structures with \( m > 4 \). When the buffer layer is present, in a some buffer thickness range the Tamm plasmon-polariton mode arises at the short-wave edge (Figure 5 a, b) and shifts to the long-wavelength edge of PBG. At the same time the alignment of microcavity and Tamm plasmon-polariton modes does not occur. But at the closest approach these modes are spectral dependent. That is, the modes have a similar line-shape and behave the same way with the change of \( m \). When \( m = 4 \) for both modes the sign inversion of peaks takes place (Figure 5 c, d). Thus, as shown by the results, to achieve the highest angles of rotation of light polarization plane in reflection the using of 1D-PC with Tamm plasmon-polariton mode is not profitable.
Figure 5. Spectra of polar Kerr rotation $\Theta_K$ of model 1D-PC with MA defect of $(\lambda_0/2)$-optical thickness for I microcavity mode and controlled by the thickness of buffer layer $h_{\text{SiO}_2}$. Tamm plasmon-polariton mode as a function of the number $m$ at unchanged thickness of top gold layer $h_{\text{Au}} = 200$ nm.

4. Summary
The modelling of polar Kerr rotation spectra of one-dimensional photonic crystal with highly Bi-substituted iron garnet defect and top buffer SiO$_2$ and gold layers of different thicknesses demonstrates a strong dependence of spectral line-shapes of microcavity and Tamm plasmon-polariton modes on number of layer pairs $m$. In the vicinity of $m = 4$ or $m = 5$ the signs of the peaks of both modes inverse as mode approach to each other. Similar occurs for only one microcavity mode, if modes spectrally separated. The modification of the spectral dependences caused by the large absorption of highly Bi-substituted iron garnet defect. In order to enhance the magnetooptical response in reflection geometry is better to use only one top gold layer without a buffer layer. The maximum of polar Kerr rotation $\Theta_K = 21.3$ deg have the structure with $m = 5$ and amplification effect is 4 times as compared with the structure without gold.

Acknowledgments
This work is supported by the RF Ministry of Education and Science in the framework of the base part of the state task №2015 / 701 (project 3879).

References
[1] Inoue M, Baryshev A V, Goto T, Back S M, Mito S, Takagi H and Lim P B 2013 Magnetophotonics (Springer-Verlag Berlin Heidelberg)
[2] Berzhansky V N, Mikhailova T V, Karavainikov A V, Prokopov A R, Shaposhnikov A N, Kharchenko Y M, Lukienko I M, Miloslavskaya O V, Kharchenko M F, Belotelov V I and Golub V O 2015 Solid State Phenomena 230 241
[3] Kato H, Matsushita T, Takayama A et al. 2004 J. Magn. Magn. Mater. 272–276 e1305
[4] Kato H and Inoue M 1997 J. Appl. Phys. 81 5659
[5] Yin C P, Wang T B and Wang H Z 2012 Eur. Phys. J. B 85 104