Conference materials UDC 535-15 DOI: https://doi.org/10.18721/JPM.153.336

Peculiarities of the luminescence response of two-dimensional photonic crystals with ordered Ge(Si) nanoislands obtained using different ordering approaches

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Abstract. In this work, we investigated the luminescent properties of two-dimensional photonic crystals (PhCs) with ordered Ge(Si) nanoislands obtained using one- and two-stage approaches to ordering. The features of the luminescent response of such structures and their relationship with the ordering processes of nanoislands are considered. It is shown that the incorporation of Ge(Si) nanoislands into a two-dimensional PhC makes it possible to increase the intensity of their luminescent response by more than an order of magnitude, which makes the structures under consideration promising for practical applications.

Keywords: photonic crystals, Ge(Si) nanoislands, ordering, photoluminescence

Funding: Project FASO No. 0030-2021-0019 and No. FWGW-2022-0011

Citation: Peretokin A. V., Stepikhova M. V., Novikov A. V., Smagina Zh. V., Dyakov S. A., Peculiarities of the luminescence response of two-dimensional photonic crystals with ordered Ge(Si) nanoislands obtained using different ordering approaches. St. Petersburg State Polytechnical University Journal. Physics and Mathematics, 15 (3.3) (2022) 188–193. DOI: https://doi.org/10.18721/JPM.153.336

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Материалы конференции УДК 535-15 DOI: https://doi.org/10.18721/JPM.153.336

Особенности люминесцентного отклика двумерных фотонных кристаллов с упорядоченными наноостровками Ge(Si) полученных с использованием разных подходов к упорядочению

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Аннотация. В работе изучены люминесцентные свойства двумерных фотонных кристаллов (ФК) с упорядоченными наноостровками Ge(Si), полученных с использованием одно- и двухстадийного подходов к их упорядочению. Рассмотрены особенности люминесцентного отклика таких структур и их взаимосвязь с процессами

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упорядочения наноостровков. Показано, что встраивание наноостровков в двумерный ФК позволяет более чем на порядок величины увеличить интенсивность сигнала ФЛ.

Ключевые слова: фотонные кристаллы, наноостровки Ge(Si), фотолюминесценция

Финансирование: Государственное задание темы № 0030-2021-0019 и № FWGW-2022-0011.

Ссылка при цитировании: Перетокин А. В., Степихова М. В., Новиков А. В., Смагина Ж. В., Дьяков С. А., Особенности люминесцентного отклика двумерных фотонных кристаллов с упорядоченными наноостровками Ge(Si), полученных с использованием разных подходов к упорядочению // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2022. Т. 15. № 3.3. С. 188–193. DOI: https://doi.org/10.18721/ JPM.153.336

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Introduction

Today, the problem of creating efficient radiation sources for optical connections in the processor architecture remains unsolved [1]. Such connections will reduce the power consumption of processors and increase the speed of information processing. One of the main requirements for sources is their technological compatibility with silicon, which, as is known, is the main material of microelectronics, however, due to its indirect band gap, it has poor emitting properties.

Ge(Si) nanoislands are one of the options for such radiation sources, having a number of significant advantages: they are compatible with CMOS technology [2]; emit in the wavelength range of $1.2-1.6 \mu m$, which is the main one for telecommunication systems [3]; they are relatively easy to produce and compact [2]; and, what is important in this work, there is the possibility of their spatial ordering on a silicon substrate [4]. The main disadvantage of Ge(Si) nanoislands is their relatively low emissivity. In order to increase the radiative efficiency of nanoislands, various options for their incorporation into low-dimensional cavities are currently being considered [5].

A large number of works [6] are devoted to photonic crystal cavities, in which an increase in the photoluminescence (PL) intensity of nanoislands is observed, reaching more than an order of magnitude, and the quality factor of the observed resonances exceeds 10⁴. It was shown that due to the precise embedding of the nanoislands in the maximum of the cavity mode field, it is possible to achieve an even higher signal amplification [6]. However, such structures have a small emitting volume and require high manufacturing precision, therefore it is much more profitable to use photonic crystals (PhCs) themselves, without a cavity, where all nanoislands are involved in the radiation processes, and not just those located in the small cavity.

For PhCs, it is also natural to think about the possibility to increase the amplification of nanoislands luminescence response due to their precise incorporation into field maxima of PhC modes. However, to date there is only one work where this idea was discussed [7], i.e., this task remains relevant.

Materials and Methods

The samples grown on SOI substrates with a Si layer thickness over the oxide of 80–90 nm were studied. For the ordered growth of nanoislands, the preliminary formation of seed pits in the substrate was used [4]. It's known that, depending on the parameters of the pits and the parameters of the formed lattice, the nucleation of nanoislands can occur both inside the pits and around them [8]. Therefore, two approaches to the nanoislands ordering in a PhC are possible: two-stage and one-stage.

To analyze the features of both approaches, 2 samples were grown. The first one was obtained using the classical two-stage ordering approach. With this approach, the fabrication of a sample occurs in two stages: I) – formation of an array of spatially ordered Ge(Si) nanoislands, and II) – formation of a PhC. At the first stage, square arrays of shallow, small in size, seed pits with a period of $1-4 \mu m$ were created on the substrate. Next, 4.5 Ge monolayers were deposited by

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molecular beam epitaxy (MBE), forming Ge(Si) nanoislands inside the seed pits. Then, a silicon layer 15 nm thick was deposited by the MBE method, and a layer of nanoislands was again grown. The silicon thickness of 15 nm ensured the vertical ordering of nanoislands in the direction of growth. Thus, a structure with 10 layers of Ge(Si) nanoislands was obtained, with a total thickness above the oxide layer of ~ 300 nm; the upper layer of nanoislands was not overgrown for visual control of nanoislands location. At the second stage, in the obtained multilayer structure, in regions with ordered nanoislands, PhCs with a hexagonal lattice of holes were formed, with periods $a = 525 \div 600$ nm and the ratio $r/a = 0.14 \div 0.17$ (where r is the radius of the holes), the depth of the holes was ~ 220 nm. The growth technology and the fabrication process of this sample are described in more detail in [9].

In the one-stage approach to the nanoislands ordering, deep seed pits with vertical walls etched through the entire thickness of the active layer were used. Arrays of seed pits 200 nm in diameter were formed, arranged in a square lattice with a period of 500-2000 nm. Further, as in the previous case, a multilayer structure was grown with 4 layers of Ge(Si) nanoislands, with a total thickness of ~ 255 nm above the oxide layer. In contrast to the previous structure, the ordering of nanoislands in this case occurred around seed pits or between them. Under certain conditions, during growth, such pits did not overgrow, acting as holes of the PhC. The process of formation of such a sample is described in more detail in the article [10].

The studies in this work were carried out using a standard micro-photoluminescence (micro-PL) technique, which provides the possibility of measurements with high spatial (up to 2 μ m) and spectral (up to 0.01 cm⁻¹) resolution [11]. All measurements were performed at a temperature of 77 K. The PL signal was excited by a solid-state laser with a wavelength of 532 nm, the laser power was varied from 3 to 4 mW.

The theoretical analysis of the formed PhCs was performed by the Fourier modal method in the scattering matrix formalism [12].

Results and Discussion

Fig. 1, *a* shows: the micro-PL spectra of PhC obtained using the two-stage approach, and, for comparison, of the initial, unprocessed region of the sample, without ordered Ge(Si) nanoislands. PhC period was 525 nm, r/a = 0.17. PhC was formed in the ordering region of nanoislands with a period of 1µm. For this PhC, the maximum enhancement (η) of the luminescent response of Ge(Si) nanoislands was observed. At the maximum, PL signal increased almost 40 times, with respect to the signal measured in the unprocessed sample region, the increase in the integral intensity of the signal exceeded an order of magnitude ($\eta_{integral} = 12$). This enhancement of PL signal is explained by the interaction of Ge(Si) nanoislands with the optically active PhC modes, as evidenced by the presence of narrow peaks in the PL spectrum. As we showed earlier, the formation of photonic crystals in regions with long ordering periods of Ge(Si) nanoislands leads to a weaker increase in signal intensity, which is explained by a decrease in the surface density of nanoislands and, as a consequence, the number of ones interacting with PhC modes and contributing to PL signal [9].

The micro-PL spectrum of photonic crystal obtained using the one-stage approach is shown in Fig. 1, *b*, period of PhC is a = 700 nm. For the PhC presented, the maximum enhancement of luminescence response related with Ge(Si) nanoislands was observed. As in the two-stage approach, PL signal of photonic crystals obtained by this method exceeded by an order of magnitude the signal observed in the unprocessed region ($\eta_{peak} = 12$). The main feature of these PhCs is the strong dependence of their luminescence properties on the conditions of nanoislands formation. As the results of studies have shown, in photonic crystals with a small lattice period, under the growth conditions used, Ge(Si) nanoislands are not formed and have poor radiating properties. At large lattice periods of PhCs, nanoislands turned out to be completely formed, but the spectral range of their emission began to overlap with the high-order PhC modes, which are characterized by the low efficiency and a high degree of degeneracy, as evidenced by low-intense PL spectra observed for such PhCs, represented by broad PL lines [10]. The most optimal in this case are the lattice periods of PhCs a = 700-900 nm.

Fig. 2 shows the results of numerical simulation of the dispersion characteristics of emissivity carried out for the studied PhCs and the calculated field patterns of the most intense modes. The results of numerical simulation show that in PhCs with a hexagonal lattice of holes obtained by



Fig. 1. Micro-PL spectra of photonic crystals obtained using (*a*) two- and (*b*) one-stage approaches to the ordering of Ge(Si) nanoislands. For comparison, in both figures, the micro-PL spectra of the original, unprocessed regions of the corresponding sample are shown in dark gray. The insets to the figures show SEM images of the studied PhCs. The values η_{peak} and $\eta_{integral}$ are the PL signal amplification at the maximum and the integral signal amplification observed in the PhCs compared to the signal in the initial unprocessed region of the sample

the two-stage method, the most intense PL line corresponds to the doublet E_2 mode [11], which is characterized by the presence of a symmetry-protected bound state in the continuum (BIC) at the Γ point of the Brillouin zone (Fig. 2, *a*). The emission maximum of this mode, observed in experiment, turns out to be shifted to the region of large wave-vectors in the Γ -K direction nof the Brillouin zone, which may be due to the shallow depth of the holes formed in these PhCs. In a PhC with a square lattice obtained by a one-stage method, the most intense line in PL spectrum is represented by two closely spaced singlet modes A_2 and B_2 , which also show the features of BICs (Fig. 2, *c*). The bound-states in the continuum are characterized by a discontinuity in the dispersion curves of the emissivity at the Γ point, as it follows from the numerical simulation data (Fig. 2, *a*, *c*), and by extremely high values of the quality factor when compared with conventional radiative modes [12, 13].



Fig. 2. Results of numerical simulation of the emissivity of studied PhCs near the Γ -point of Brillouin zone (*a*, *c*). The calculations were performed for PhCs shown in Fig. 1. The asterisks mark position of the maximum of PL signal observed in the experiment. The blue lines in the figures indicate emission range of the nanoislands, green lines indicate the collection angles of PL signal. Are the results of numerical simulation of field distribution carried out for PhC modes (*b*, *d*), indicated by asterisks in figures (*a*, *c*), respectively. The green circles indicate position of PhC holes, the blue circles in Fig. (*d*) indicate location of Ge(Si) nanoislands

Analyzing both approaches used in this work to the ordering of Ge(Si) nanoislands in photonic crystals, and considering the possibilities of embedding nanoislands in the maxima of the field of PhC modes, let us focus on the following. As mentioned above, in the two-stage approach, the ordering of nanoislands and the formation of PhCs occur at different stages, which makes it possible to form PhCs with any parameters and good hole quality, since this technology is well developed.

However, the main limitation here is the size of the nanoislands formed and the values of the minimum periods at which their ordering is possible. As follows from the field simulations carried out for the most intense mode (Fig. 2, *b*), it is optimal to build nanoislands between PhC holes, i.e. form a lattice of nanoislands with a period corresponding to S of PhC period, which is not feasible, since, according to literature, the minimum ordering period of Ge(Si) nanoislands is 425-500 nm [2, 4]. The incorporation of nanoislands into PhCs with a longer period should lead to a shift in the spectrum of optically active modes coinciding in energy with the emission range of Ge(Si) nanoislands into the range of high-order modes.

In the one-stage approach, due to the simultaneous formation of a PhC and the ordering of nanoislands, it becomes possible to form a PhC with any lattice parameters with ordered groups of Ge(Si) nanoislands. Ge(Si) nanoislands can be formed both around holes and between them [2, 10], which is true for square and hexagonal lattices. As can be seen in Fig. 2, d, the field distribution of the most intense mode in PhC with the square hole lattice obtained by one-stage formation method is even more complex than in the case of PhC considered in two-stage approach, however, due to the ordering of nanoislands around PhC holes, here we observe a stronger correlation in the spatial arrangement of the nanoislands with the field maxima of optically active PhC mode. Since the nanoislands are ordered in the same way around all holes, a high degree of periodicity of nanoislands incorporating into PhCs is achieved. To implement such an approach with two-stage ordering, it is necessary to separately solve the problem of combining arrays of nanoislands and PhCs, which, as discussed above, is not always possible. The main drawback of one-stage approach is the fact that during the growth process, holes that form photonic crystal can be partially or completely overgrown, due to which the PhC periodicity worsens, and, as a result, the quality factor of spectral lines. This is clearly seen in the SEM images shown in Fig. 1. Another consequence of the hole overgrowth is the small values of r/a ratio, which leads to the involvement of high-order modes in PL signal (Fig. 2, c). Nevertheless, despite such a non-ideal PhC, a spectrum of narrow lines is experimentally observed for it, exceeding the intensity of the PL signal in the unprocessed region of the sample by more than an order of magnitude.

Conclusion

As discussed above, both approaches considered by us to the ordering of Ge(Si) nanoislands in PhCs have their own advantages and disadvantages. Obviously, in order to minimize the disadvantages, it makes sense to combine these approaches: using a single-stage approach, one can achieve ordering of nanoislands between or around PhC holes, and then, using the second step from the two-stage approach, "once again" form a PhC with the same lattice parameters, but with better hole settings. Thus, it can be assumed that it will be possible to obtain a good-quality PhCs with ordered nanoislands around each hole, or between them. From the point of view of further research, here we should also once again pay attention to the two-stage approach, bearing in mind the possibility of combining the ordering lattices of Ge(Si) and PhC nanoislands. For the same (or multiple) periods of the lattices, it is possible to consider the possibility of their different mutual arrangement, which makes it possible to embed nanoislands in the selected PhC regions, maximally matching their position with the field maxima of the electromagnetic modes. Such studies can give a deeper understanding of the nanoislands interaction processes with PhC modes and of the ordering effects of nanoislands in PhCs on their luminescence response.

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Received 08.08.2022. Approved after reviewing 11.08.2022. Accepted 30.08.2022.