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Silicon nitride photonic crystal cavity coupled with NV-centers in nanodiamonds

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Abstract

The development of integrated quantum photonics requires a high efficient excitation and coupling of a single photon source with on-chip devices. In this paper, we show our results of modelling for high-Q photonic crystal cavity, optimized for zero phonon line emission of NV-centers in nanodiamonds. Modelling was performed for the silicon nitride platform and obtained a quality factor equals to 6136 at 637 nm wavelength.

Keywords: Photonic crystal cavity; Nanophotonics; NV-centers; Silicon nitride

1. Introduction

Nowadays integrated photonics is a very promising field of study. It has such advantages as possibility to create devices with a small footprint, to combine different devices together on a single chip and easy scalability. Integrated photonics can be realized with different materials, including silicon-on-insulator (SOI), silica (SiO_2), lithium niobate-on-insulator (LNOI), A_3B_5 – materials, silicon nitride (Si_3N_4) and others. All of them have their own advantages and disadvantages, and today it is difficult to find a platform suitable for all potential applications. Usage of silicon nitride platform here looks really good due to its properties, like transparency in wavelength range of interest, low losses in material and well developed fabrication processes.

The relatively new part of integrated photonics is quantum integrated photonics (QIP). Along with single-photon detectors, logical gates, QIP requires a single-photon source of light. This field has great prospects in developing of quantum communications, data analysis, simulation and computing (O'Brien, Furusawa, and Vučković, 2009). One of the most important step on a way toward to fully integrated on-chip devices is a high-efficient coupling between single-photon source and photonic circuit.

At present, no ideal single-photon source has yet been found, therefore, work is being carried out in parallel with different quantum objects. The most convenient for on-chip integration single-photon sources are quantum dots, carbon nanotubes, and color centers in diamonds (Aharonovich, Englund, and Toth, 2016). NV-centers in nanodiamonds are an interesting candidate on this role, due to their optical and spin coherence properties (Jelezko and Wrachtrup, 2006).

The drawback of single NV-center is small number of photons (about 3%) coherently emitted in the zero-phonon line, highly reducing emission rate of the source. To increase the emission efficiency by putting the NV-center into the photonic cavity, the Purcell effect may be used. Efficiency increases directly proportional to the Quality-factor of the resonator (Purcell, 1946). For this reason, using an on-chip photonic cavity the two important problems: increasing the single-photon efficiency generation, as well as significant coupling with waveguide can be simultaneously solve.

Such an approach was shown recently (Fehler et al., 2019) for the Si_3N_4 platform, providing high efficiency for 762.1 nm wavelength, using a photonic crystal cavity (PhC). The silicon nitride platform was chosen due to low losses in the visible wavelength range and well-developed CMOS fabrication process. Despite the integrated approach, demonstrated in the article, the resonant wavelength of the PhC did not matched the zero-phonon line of the NV center, equals to 1.945 eV (637 nm at wavelengths) and further optimization is still needed.

In this work, we performed modeling of the PhC, to optimized resonance wavelength for zero-phonon line NV-center emission.

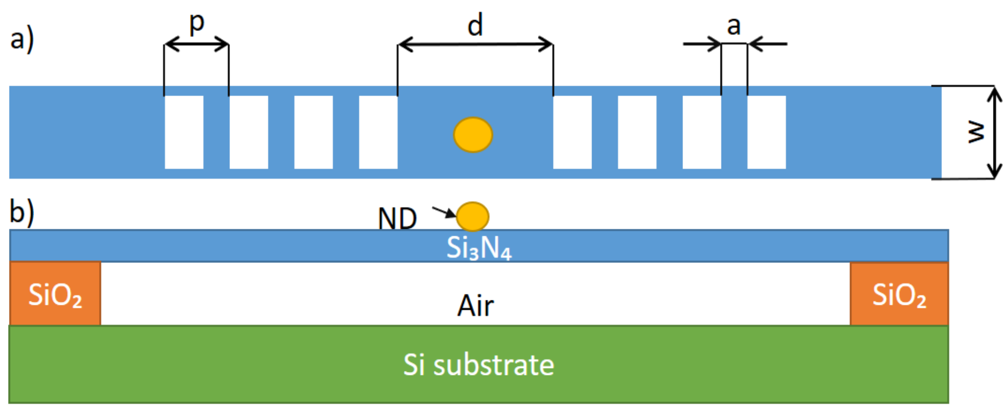

Figure 1. Schematic view of PhC with nanodiamond atop (ND); top (a) and side (b) view.

Our results have a great potential for increase the total on-chip efficiency of NV-center atop silicon nitride waveguide.

2. State-of-art

There are already developed different types of PhC for enhancement of a single-photon sources emission rate throw Purcell effect. In recent research efficient PhC for NV-center at 762.1 nm wavelength was shown (Fehler et al., 2019). This work demonstrates design for PhC with circular holes and successful practical realization. Authors demonstrated Q-factor up to 51,000 at Si_3N_4 platform.

In the same way PhC for SiV-centers in diamond were calculated and fabricated (Fehler et al., 2020). Here fabricated device had Q-factor equals to 1000 for ZPL of SiV-center.

The similar design of PhC, but optimized for ZPL of NV-center also was shown recently (Olthaus, Schrinner, Reiter, and Schuck, 2020). Authors also used a silicon nitride platform for device developing. This work demonstrates maximum Q-factor up to 2×10^5 and 4.5×10^3 for the calculated and the fabricated device, respectively. Such a huge value was for number of mirror segments large enough for saturation of Q-factor, that means transmission losses were switched off. These works shown that such way of enhancement single-photon emission rate is a quite efficient and useful.

Here, we suggest a different design of PhC, which is easier for development, but comparable by efficiency. Similar design was studied for diamond platform based PhC (Li, et al., 2015), which we used as a starting point.

3. Materials and Methods

We chose the photonic layers' thicknesses based on our previous experience with commercially available Si wafers, thermal oxidized layer of SiO_2 (2μm) and Si_3N_4 atop (200 nm). Here the silicon oxide layer is a separator for silicon nitride from silicon. This separation is important, because it produces a higher refractive index contrast around Si_3N_4 layer. Thicknesses of layers were optimized to increase efficiency of focusing grating couplers (FGCs), due to reflection from the silica-silicon interface (Mehta and Ram, 2017). Waveguide width and height were optimized for working at fundamental TE mode of electromagnetic radiation in wavelength of interest.

PhC was designed as a planar ridge waveguide with etched rectangular holes, acting as a semi-transparent mirror along waveguide axis (Figure 1, a). The width of the holes is a 60 nm less than the waveguide width. This was invented for further possibility of SiO_2 wet etching in hydrofluoric acid (Havereke, et al. 1994), to create free standing cavity. This approach should increase PhC's Q-factor. The resonant cavity is a part of waveguide in the center, surrounded on both sides by the holes. Period of holes denoted as p, distance of cavity as d, width of waveguide as w and width of Si_3N_4 between two neighbor holes as a. Also we determined filling factor as $ff = a/p$.

In this work, we performed 2D modelling according finite difference time domain (FDTD) method, using free and open-source MEEP library in Python, as well as finite element method (FEM) implemented in COMSOL Multiphysics software. FEM was used to determine modes of radiation propagation in cross-section of the studied waveguide. FDTD method was used for calculations of quality-factor and transmission for PhC. This method is convenient for similar tasks and was used in all papers mentioned in state-of-art section.

4. Modelling

At first, the width of Si_3N_4 waveguide was chosen as 450 nm, to match the fundamental transverse-electrical mode close to the 637 nm wavelength. Such a result was obtained from numerical calculation of waveguide's cross-section (Figure 2 a, b) using FEM in COMSOL Multiphysics software.

After that, we started to study the 2D model of the PhC using MEEP. In Figure 2c. an example of electric field distribution is shown. For the model resolution equals to 100 pixels/μm was chosen, due to the minimal elements of a model have smallest size equals to 30 nm. Cladding and holes were filled with air layer (n=1), while for the core we used silicon nitride refractive index equals to 2.01 for 637 nm wavelength. For the quality factor calculation, we placed a dipole, acting as a photon source in the middle of the cavity (Figure 1, a, b). The whole model was surrounded by perfectly matched layer (PML) for avoiding reflections from the boundaries.

Later we varied period and filling factor of the holes to obtain a maximum transmission and Q-factor at 637 nm wavelength. Number of periods was equal to 51 for each segment of mirror. As a result of this modelling we plotted a color contour map where color codes a wavelength, as well as x, y-axes correspond to filling factor and period (Figure 3a). After that in our data points, closest to the line of 637 nm we calculated transmittance and Q-factor (Figure 3b). Then we studied dependence of Q-factor on the cavity distance (Figure 3c).

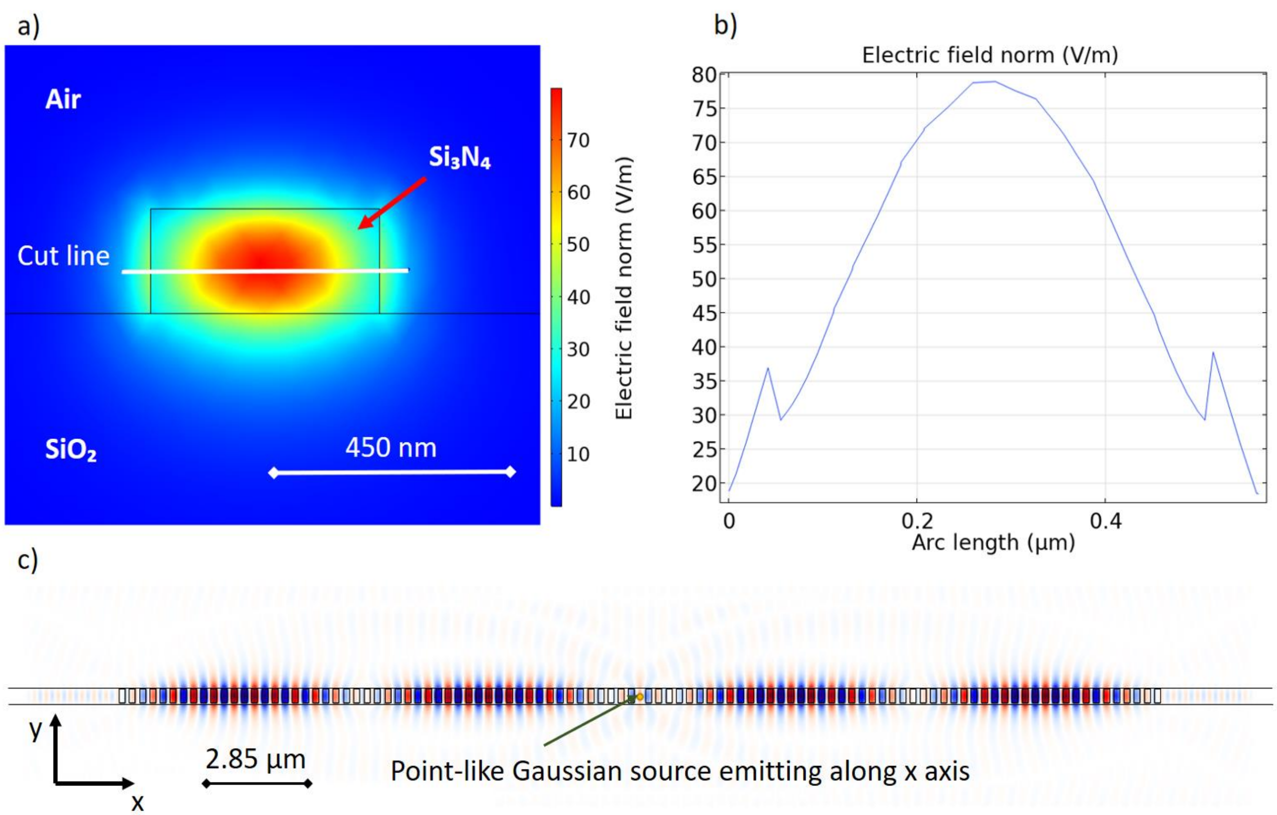

Figure 2. a) Electric field distribution inside cross-section of silicon nitride waveguide. b) Electric field distribution in waveguide along cut line. c) Distribution of y-component of electric field in PhC with a point-like Gaussian source in the middle.

5. Results and Discussion

At first, from color contour map (Figure 3a) we obtained that resonant wavelength depending on both filling factor and period, as well as this dependence fitted by the line. Qualitatively, this can be explained as follows. With an increase in the period, according to the Bragg condition, the wavelength increases. With an increase in the filling factor, due to an increase in the effective refractive index, the wavelength also shifts towards longer wavelengths. For this reason, it's possible to find conditions, when the same wavelength can be obtained by a different combination of period and filling factor.

Then, we took several points with the resonant wavelength conditions closest to 637 nm from this contour color map, and compared transmission and Q-factor of each point. We found that despite the fact that different combinations of filling factor and period gave the same wavelength of 637 nm, both transmission and Q-factor was different in each point (Figure 3b).

After analysis of the Figure 3b, we chose as the most promising couple of parameters: filling factor equals to 0.4 and period equals to 280 nm. For such values the resonant wavelength was equal to 626 nm, Q-factor equals to 4880 and transmission equals to 0.55. For adjusting of resonant wavelength we increased period till 285 nm. This change also affected Q-factor and transmission and tuning values of 4691 and 0.41 respectively. After that, we changed the cavity distance to maximize cavity Q-factor (Figure 3c). Obtained optimal distance of the cavity was equal to 320 nm. From this optimization we increased Q-factor up to 6136 and transmission value up to 0.5.

Thus, we numerically obtained parameters for the PhC cavity at a wavelength range close to 637 nm, including filling factor (0.4), holes periodicity (285 nm) and cavity width (320 nm). We also studied the influence of a difference in width between holes and waveguide on properties of silicon nitride PhC and found that small difference has a small influence on transmission and Q-factor, but further increasing of this value will significantly decrease Q-factor of the PhC. The cavity transmittance of 0.5 and Q-factor equals to 6136 (Figure 3d) for the optimized parameters, were found.

Obtained results characterize the studied PhC as fitted for the fabrication and integration with real NV-centers in nanodiamonds atop of the cavity.

6. Conclusions

We performed a numerical analysis and obtained the PhC parameters for the efficient integration of NV-centers in nanodiamond and silicon nitride circuits. We performed 2D modelling so accuracy of our results restricted by this fact. However, it is enough for estimation of the main parameters of the PhC and results presented in this paper can be used for fabrication of the PhC optimized for 637 nm wavelength. Usage of such PhC can significantly increase efficiency of NV-center in nanodiamond as a single-photon source. Integrated quantum photonic circuits have different applications in quantum communications, including quantum memory (Li, et al., 2015) and quantum gates (Su, et al., 2008).

Our further studies will focus on the use of a 3D model, as well as PhCs practical implementation and their experimental study.

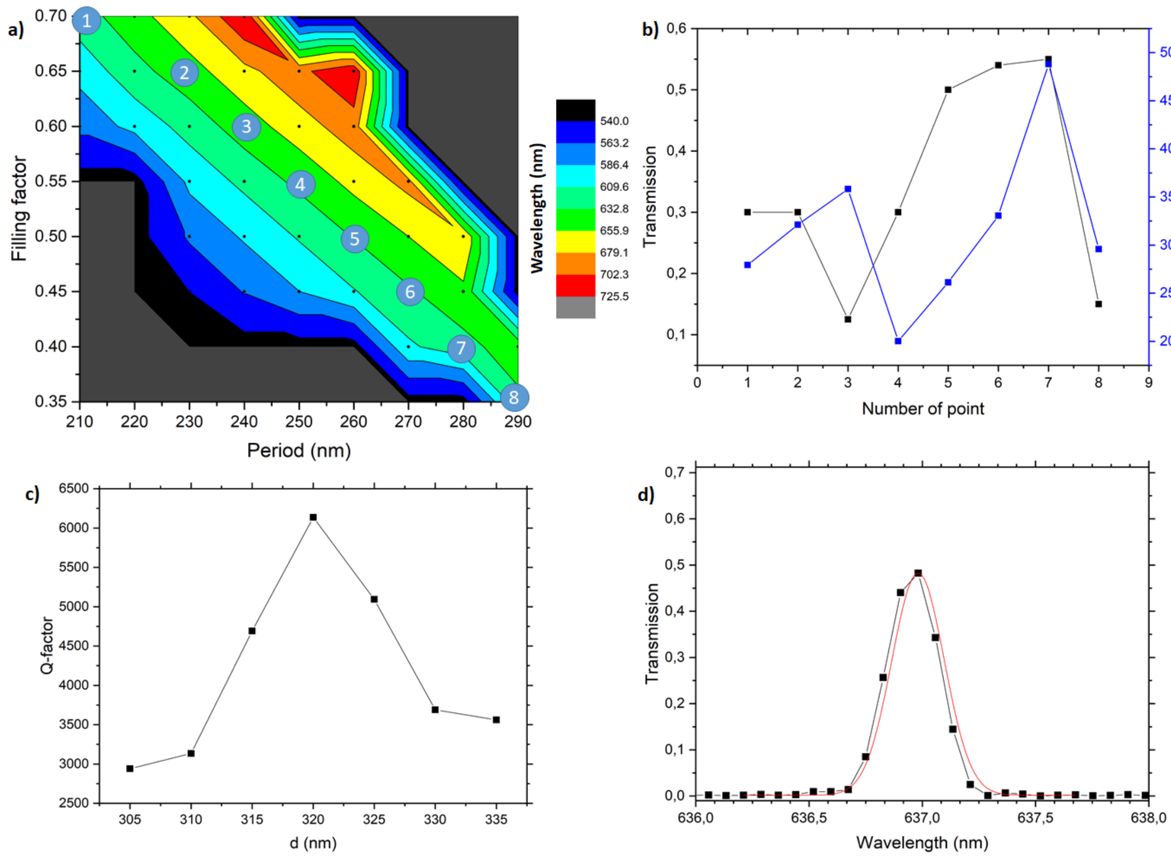

Figure 3.a) Color map shows dependence of resonant wavelength from period and filling factor with numerated points for graph b. b) Q-factor and transmission along the line of data from color map which has resonant wavelength closest to 637 nm c) Q-factor with respect to cavity distance d d) Transmission for best parameters with Gaussian fitting (red line)

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References

Aharonovich, I., Englund, D. & Toth, M. (2016). Solid-state single-photon emitters. *Nature Photon* 10:631–641

Fehler, K. G. et al. (2019). Efficient Coupling of an Ensemble of Nitrogen Vacancy Center to the Mode of a High-Q, Si3N4 Photonic Crystal Cavity. *ACS Nano*, 13 (6):6891-6898

Fehler, K. G. et al. (2020). Purcell-enhanced emission from individual SiV- center in nanodiamonds coupled to a Si3N4-based, photonic crystal cavity. arXiv:1910.06114

Havereke, S. et al. (1994). The etching mechanisms of SiO2 in Hydrofluoric acid. Journal of The Electrochemical Society. 141: 2852

Jelezko, F., Wrachtrup, J. (2006). Single Defect Centres in Diamond: A Review. *Phys. Status Solidi A*, 203:3207-3225.

Li, L., et al. (2015). Coherent spin control of a nanocavity-enhanced qubit in diamond. *Nat Commun* 6:6173.

Mehta, K.K. and Ram, R.J. (2017). Precise and diffraction-limited waveguide-to-free-space focusing gratings. *Sci Rep*, 7:2019

O'Brien, J. L., Furusawa, A., and Vučković, J. (2009). Photonic Quantum Technologies. *Nature Photonics*, 3.12:687–695.

Olthaus, J., Schrinner, P.P.J., Reiter, D.E. and Schuck, C. (2020). Optimal Photonic Crystal Cavities for Coupling Nanoemitters to Photonic Integrated Circuits. *Adv. Quantum Technol.*, 3: 1900084.

Purcell, E. M. (1946). Spontaneous emission probabilities at radio frequencies. *Phys. Rev.*, 69:681

Su, C.-H., et al. (2008) High-Speed Quantum Gates with Cavity Quantum Electrodynamics. *Phys. Rev.*, A 78:062336