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Photonic crystal nano-cavities for enhancing zero-phonon line emission from nitrogen-vacancy centers in diamond

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ABSTRACT

This paper presents designs of nano-cavity structures based on a photonic crystal in diamond in order to achieve high-efficiency collection of zero-phonon line (ZPL) photons emitted from the nitrogen-vacancy centers in diamond. The cutoff radius is calculated so as to ensure that the dual-resonances for both the pump and the ZPL photons could exist in the designed cavities. Our conceptual designs are demonstrated through simulations by finite-difference time-domain (FDTD) method. High Q for the pump ($\sim 1.9148 \times 10^5$), strong enhancement of spontaneous emission in terms of Purcell factor ($\sim$3812.1), and high coupling efficiencies for pump and for ZPL output ($\sim$94.06% and 92.19% respectively) could be numerically obtained, which may make our designs applicable in quantum-optical information processing systems such as quantum nodes or quantum repeaters.

1. Introduction

Photonic crystals (PhCs), which normally contain two kinds of dielectric materials distributed periodically in space, have attracted a lot of attention. PhCs can basically serve as "semi-conductors" to photons. Micro-cavities made of PhCs can achieve strong localization of photons; as a result, a high quality factor Q and a small mode volume could be obtained in PhC micro-cavities. Based on this principle, micro-cavities in PhCs for making strong enhancement of spontaneous emission (SE) [1–6] and stimulated Raman scattering (SRS) [7–9] have been extensively investigated.

Recently, diamond has been studied for its application in quantum-optical information processing technology [10,11], due to its attractive optical and quantum properties. In single-crystal diamond systems in which negatively charged nitrogen-vacancy (NV^-) centers are embedded, the electron spin states could be coherently and optically read out. The coupled-out photons in the proportion of zero-phonon line (ZPL) of SE are carriers of qbits, since their degrees of freedom can change with electron spin states. Under room temperature, degrees of freedom are time-averaged due to the thermal vibrations, which show no ties between the ZPL photons and NV^- spin states. At low temperatures (<10 K), thermal vibrations are suppressed which contributes to the strong interaction between the spin and orbits, resulting of spin-photon entanglement. Applying optical cavities with high Q to enhance the ZPL, the aim of generating entanglement can be achieved [11b,11c,11d,11e,11f].

Generally, there are two methods for coupling out the SE from diamond NV^- centers [12]. One way is using non-resonant collecting structures, including solid immersion lenses [13] and diamond waveguides [14]. In this case, a critical problem is how to optimize structures to increase the collection efficiency. Another method is employing resonant confining structures, such as plasmonic resonators [15–18], micro-disk cavities [19,19b], microsphere resonators [20–22] and PhC cavities [1–6].

Recently, one design which is based on plasmonic resonators for collecting the SE around 637 nm which corresponds to the ZPL, has been reported [15]. This design has an ultra-small modal volume V_m $\{\sim 0.04(\lambda/n)^3\}$ in plasmonic resonators; also it has been found that the Purcell factor, which is a measure of the spontaneous emission rate [23,24], could reach relatively high value ($\sim$50), in contrast to the result ($\sim$13) shown in Ref. [25]. Despite this, the plasmonic aperture introduces a high loss, as a resulted of the small quality factor Q ($\sim$180), which offsets the contribution from small modal volume. (Note that the Purcell factor is proportional to Q/V_m.) Meanwhile, the optimal collection efficiency ($\sim$40%) requires a 0.95 N.A. lens to collect the emitted photons, which may not be suitable for the future all-optical integrated circuits.

Barclay *et al.* reported a micro-disk system with a high Q of the order of 10^5 for the whispering-gallery mode (WGM) [19]. However, since the diamond nanocrystal which contains NV^- centers is placed on the top-surface of the micro-disk made of SiO_2, the

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perturbation to the propagation modes is inevitable; in addition, the modal volume is large $\{\sim 82(\lambda/n)^3\}$, resulting in a relatively small Purcell factor and thus weakening the enhancement of SE. It is notable that the spectral properties (i.e. spectral diffusion) of NV^- center in the nanocrystal diamond are unfavorable, which may limit its further application. Another microdisk was demonstrated in Ref. [19b]: using the single crystal diamond and following the conventional semiconductor fabrication processes, the microdisk with high Q ($\sim$4300) could be made. It is suggested that by deterministically positioning the NV^- center and eliminating strains of NV^- center in the diamond which possess higher purity, a higher Q could be achieved, which will result in greater enhancement of ZPL.

For silica microsphere resonators coupling to NV^- centers as reported, ultra high quality factor Q ($\sim 10^8$) of the whispering gallery mode could be obtained under the low temperature (6–12.4 K), the normal mode splitting could be observed, reflecting the realization of strong coupling between the NV^- center and WGM. The drawback for such experimental systems is their critical requirement for low temperature (helium gas was used for cooling) due to the narrow line-width of the resonant mode [20].

Designs of PhC cavities made of silicon nitride (SiN_x), gallium phosphide and silicon, which possess high Q and small modal volume for collecting ZPL photons, have been presented [1–4]. For example, diamond color centers could couple with the PhC cavity made of SiN_x with Q as high as 1.4×10^6 and modal volume as small as $0.78(\lambda/n)^3$ [1]. The merit of such designs is distinctive, since ultra-high Purcell factor ($\sim 10^5$) is numerically obtained. However, the output coupling efficiencies in collecting ZPL photons in the design are not discussed. Research on PhC cavities made of nanocrystalline diamond has also been reported [26]; the calculated and measured Q factors are found to be 9100 and 525 respectively, which illustrates that the nanocrystalline structure in diamond (grain boundary) may be one of the key factors to produce such large scattering loss. Interestingly, even in the design of PhC cavities made of single crystal diamond as shown in Ref. [26b], the measured Q factor ($\sim$700) still deviates greatly from the calculated value ($\sim$26000). In terms of narrowing linewidth of NV^- emission and prolonging the lifetime of spin coherence, the single crystal diamond is excellent. However, there is one principal limitation to the Q factor: radiation loss cannot be avoided because the diamond with many holes is not identical to a uniform dielectric material. In a uniform dielectric material, total internal reflection can occur, but in a dielectric material with sub-wavelength holes, radiation loss generally cannot be avoided, i.e., waves can escape to the outside through radiation of waves by the sub-wavelength holes, which are equivalent to a group of micro-antennas. Such a radiation loss may contribute mainly to the great difference between the theoretical and experimental quality factors because the total internal reflection theory disregards the infrastructure and takes the whole structure as an equivalent uniform dielectric material. So, the radiation loss greatly weakens the advantage of vertical confining effect in the air-hole-type PhCs. And thus, adopting additional confining structures to confine waves is necessary to attain high quality factors, i.e., adding additional one-dimensional PhC films on top and bottom of the dielectric-rod-type PhC slabs is acceptable.

In this paper, we propose designs of nano-cavity structures based on a diamond PhC with a hexagonal lattice structure to collect SE from NV^- centers at the ZPL and close to it. The PhCs presented are all in dielectric-rod type, which deviate from the conventional air-hole-type PhCs that can confine waves vertically through total internal reflections [26c]. Indeed, there is a disadvantage for the dielectric-rod-type PhCs since a further process is required to build one-dimensional photonic crystal films along the top and bottom sides of the dielectric-rod-type PhC to confine waves inside. However, the dielectric-rod-type PhCs have three advantages: (1) they can operate for TE waves while the air-hole-type PhCs can only operate for TM waves; (2) their quality factor is much higher than that in air-hole-type PhCs; (3) the dielectric-rod type can conveniently promise the single mode operation, whereas in the air-hole type PhCs multi-modes are commonly found [26d,26e]. So, there is still much interest in studying dielectric-rod-type PhCs.

The paper is divided into the following sections: parameters and settings for simulations are discussed in Section 2; the third section examines the model structure and the cutoff radius. Two designs are provided in Section 4 for localization of the pump and ZPL. The enhancement of SE is analyzed in terms of Q factors, modal volumes, Purcell factors and coupling efficiencies. Conclusions are provided in Section 5.

2. Simulation parameters and settings

2.1. Purcell factor (PF)

PF is the parameter for evaluating the enhancement of spontaneous emission; it can be written as [23,24]:

$$PF = \frac{3Q}{4\pi^2 V_m}\left(\frac{\lambda}{n}\right)^3 \quad (1)$$

where Q, V_m, λ and n are the quality factor, modal volume, wavelength in vacuum for the resonant mode and the refractive index of the host material, respectively.

2.2. Coupling efficiency

We need to calculate the coupling efficiencies for the input and output waveguides as shown in Fig. 1 in Section 3. The coupling efficiency is given by:

$$\eta = 1 - Q_c/Q_{unc} \quad (2)$$

$$\frac{1}{Q_c} = \frac{1}{Q_{unc}} + \frac{1}{Q_{wg}} \quad (3)$$

where Q_c is the quality factor for the coupled cavity, Q_{unc} is the quality factor for the uncoupled cavity, and Q_{wg} is that for the coupled waveguide [27].

2.3. Purcell factor (PF)

We have used *Rsoft* for setting the transformation relationship between the wavelength in the vacuum and the normalized

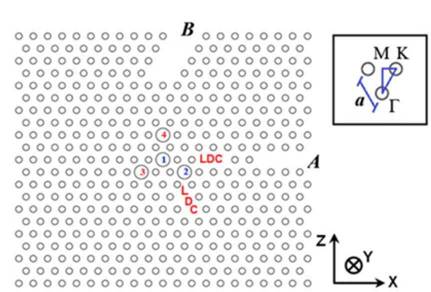

Fig. 1. Schematic of the design for collecting SE generated from NV^- color centers. Note that *A* is the input port and *B* is the output port. Rods 1 and 2 are for tuning the resonant wavelength for the pump at 532 nm, Rods 3 and 4 are for collecting ZPL photons located at the wavelength around 637 nm. The pump waves are designed to be resonant in DDC_1 and the *LDCs* nearby. The purpose of introducing DDC_2 is to increase the coupling efficiency between DDC_1 and the *LDCs*. DDC_3 and DDC_4 are designed to resonate with ZPL photons.