Diamond based photonic crystal microcavities

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Abstract: Diamond based technologies offer a material platform for the implementation of qubits for quantum computing. The photonic crystal architecture provides the route for a scalable and controllable implementation of high quality factor (Q) nanocavities, operating in the strong coupling regime for cavity quantum electrodynamics. Here we compute the photonic band structures and quality factors of microcavities in photonic crystal slabs in diamond, and compare the results with those of the more commonly-used silicon platform. We find that, in spite of the lower index contrast, diamond based photonic crystal microcavities can exhibit quality factors of $Q=3.0\times10^4$, sufficient for proof of principle demonstrations in the quantum regime.

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1. Introduction

Optical microcavities based on photonic crystal slabs have attracted much attention recently [1-11]. Almost all of these studies consider a two-dimensional photonic crystal slab (PCS) composed of a hexagonal array of cylindrical air holes in a dielectric slab. The structure is periodic in the plane and finite in the vertical direction where it is surrounded by a low index medium, usually air. The field is confined by the periodic dielectric structure in the plane and by total internal reflection (TIR) out of the plane [2]. A cavity is usually formed in either of two ways: forming a point cavity or forming a "hetero-structure". A point defect may be formed with a resonance at any frequency inside the photonic bandgap [PBG] by omitting one or more holes in the centre of the slab. [2-8]. The quality factors *(Q)* of these cavities are modest, from a few hundred to a few thousand, depending on the structure. However, the microcavity *Q* can be optimized by modifying the geometry of the lattice surrounding the cavity [2-8]. For example, Noda *et al* constructed a cavity of three missing air holes in a row of a silicon slab with hexagonal lattice structure [2] and optimized the structure by shifting neighbouring air holes outwards. Experimentally they achieved a quality factor of $Q=4.5\times10^4$, ten times higher than the quality factor of the un-optimized structure. Furthermore shifting three holes in the row next to the cavity they achieved a quality factor of $Q=1\times10^5$ [6].

High-*Q* PCS based cavities have many applications, e.g. ultra-small filters in Ref. [1] and low-threshold lasers [3]. High quality factors and small modal volume cavities are also needed to facilitate the dynamics of the strongly coupled atom-photon system for quantum information processing [8-11]. Motivated by the latter application, in this paper we choose the PCS material to be diamond, rather than the commonly used silicon or other semiconductors, since recent work has indicated that diamond is a strong candidate as a platform for Quantum Information Technology (QIT). For example, coherent oscillations and quantum beats between electron spin transitions have been observed, and a two-qubit conditional quantum gate was demonstrated using the nitrogen-vacancy (N-V) color center in diamond [12-15].

N-V centers in unstructured diamond have already been proposed as qubits in a quantum computer [16]. The method uses an ensemble of spectrally-resolved N-V centers randomly distributed in the bulk of a piece of crystalline diamond. The diamond crystal is placed between two mirrors (a "classical" Fabry-Perot resonator) to form a cavity mode around each

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N-V center. The addressing is performed by optical beams, but in this proposed scheme, it seems rather difficult to construct an optical cavity that provides photon lifetimes sufficiently long to have each N-V center coupled to the optical field in the strong coupling regime. Among other factors, Fresnel losses at the diamond faces may degrade drastically the cavity *Q*-factor.

The quality factors needed for quantum computing depend on the particular approach that is considered, varying between low values in non-deterministic schemes [17-18], to higher values in schemes that involve strong coupling. For example, estimates show that *Q* values of $Q\sim10^5$ are desirable for QIT experiments in the PCS microcavities proposed by Greentree *et al* in Ref. [19]. However, as pointed out by these authors, proof of principle experiments will be possible with significantly lower *Q* values. One problem common to most coupled atom-photon experiments for QIT is that the main decoherence channel is the bus that couples the different subsystems, which is strongly perturbed by the environment. If the qubit is localized in an ultra-high-*Q* cavity, say $Q\sim10^5$, there is a difficulty in out-coupling the excitation from the cavity. However, in a photonic crystal cavity, the possibility exists to hold photons in a high-*Q* localized mode until a control device changes the cavity from high *Q* to low *Q* (a *Q*-switch) [19]. With this "quantum gate for *Q*-switching" one can maintain high coherence until the cavity *Q* is deliberately lowered for read-out of the optical mode. Even though there have been experimental demonstrations of fairly efficient coupling to high-*Q* cavities such as in Ref. [20], the total fiber-to-cavity efficiency needs to be close to 100% for QIT experiments, and this is best accomplished by an active out-coupling.

Thus, the system under study in the present paper is a photonic crystal geometry in the single crystal diamond substrate with an array of single defects forming microcavities. In the final embodiment, single N-V centres will be placed in the defect microcavities, resonant with the N-V centre transition [19]. For this particular application, the slab geometry is convenient, since it allows the addressing of individual cavities by DC electrical fields applied from above. Such fields would be used to tune the emission of the individual N-V centre to the cavity resonance frequency. As diamond has a lower refractive index than semiconductors [22], it is unclear if sufficiently high quality factors can be obtained within a small modal volume cavity in diamond-based PCS. To resolve this question, we have explored a number of different *point cavity* designs. In this paper we only present designs that yield the highest *Q*s within a modal volume of order one cubic wavelength. We compare the *Q* that can be obtained to that in silicon that has a refractive index n=3.4 that typical for semiconductors.

Our design procedure consists of two steps: We first determine PBGs of diamond based crystal slabs and compare them with PBGs of the silicon PCS. Subsequently, we evaluate quality factors of microcavities in diamond-based PCS.

2. PC geometry and method

The model is a PCS composed of a hexagonal array of cylindrical air holes in a dielectric slab, [see Fig. 1(a)]. Diamond has smaller refractive index, *n=2.4*, than semiconductors, leading to weaker TIR guidance in the vertical direction and a cavity mode that is less well confined in the vertical direction. .

We consider two cavities. One cavity is formed using one missing hole in the centre of the slab, as illustrated in Fig. 1(a). The regular structure has holes of radius *R*, with *a* the lattice constant. In Fig. 1(b), modifications to the holes surrounding the cavity are illustrated. Neighbouring holes above and below the cavity have a reduced radius *r*. The air holes in the *x*-direction are shifted outwards by a distance *d*. This type of the cavity modification, but in a silicon PCS, was first described by Zhang *et al* [7]. The second cavity, shown in Fig. 1(c), is formed by three adjacent missing holes. Following Akahane *et al* [6], the structure is optimized by outward shifting of the left and right air holes in the row next to the cavity.

The plane wave expansion method (PWE) is used to calculate the photonic band gaps in Section 3.1 and the three-dimensional finite-difference time-domain method (FDTD), and

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Padé approximation with Bakers algorithm, are used to determine the quality factor of the cavity in Section 3.2 [23]. The modal volume is calculated using: $\iiint UdV \Big/ \max(U)$ where $U = \varepsilon |E|^2 / 2$ is the electric energy density [7].

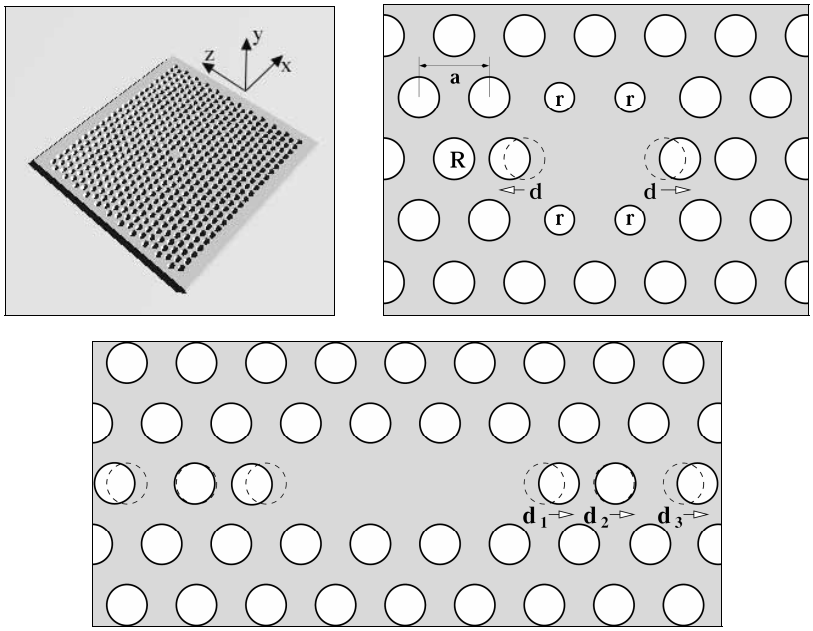

Fig. 1. (a) Schematic of bulk photonic crystal slab (PCS) and modifications of the geometry around the cavity described (b) by Zhang *et al* in Ref [7] and (c) by Song *et a*l in Ref. [6].

In our design we first choose the parity of the dominant field component in the slab with respect to the mirror plane parallel to the slab, the thickness of the slab and radius of the holes for the bulk PCS without a cavity. Once the bulk parameters are optimized, we introduce the cavities. We then optimize the quality factor by modifying the geometry of the holes neighbouring the cavity [2, 7].

3. Results

3.1 PBG calculations

We start with a PCS structure that is infinite in the plane and finite in the vertical direction, surrounded by air. The total quality factor, Q, can be separated into the in-plane value, $Q_{//}$, and out-of-plane value, $Q_{\perp}$. $Q_{//}$ can, in principle, be made arbitrarily high by increasing the number of periods. As the vertical confinement is ruled by TIR, the out-of-plane factor is crucial in designing high quality factor cavities [4]. As the structure has symmetry in the vertical direction, its modes may be classified as even or odd with respect to the parity of the dominant field component, E_x. These modes have different bands and band gaps and the vertical radiation losses can be significantly reduced by choosing modes of a specific parity [5]. Even modes were chosen because the first gap appears at lower frequencies than that for the odd modes.

We begin by selecting the properties of the bulk lattice. In Fig. 2, we show reduced band diagrams that carry information needed for the optimization: the width and relative frequency of the gap. The width and fraction of the band gap below the light line are important indicators

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in the optimization of the cavity, since frequency gaps tend to have high $Q_{\perp}$, and wide gap tend to have high $Q_{//}$ [4, 24]. In order to obtain a large fraction of the PBG below the light line the first gap should occur at the lowest possible frequency.

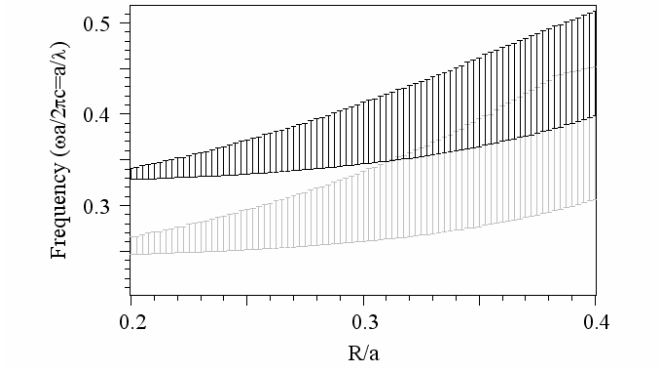

Fig. 2. Lowest photonic band gap as a function of the relative hole radius of even parity fields for silicon (grey) and diamond (black).

Diamond permits slabs that are thicker than silicon, due to the smaller refractive index. In Fig. 2 the thickness is fixed for both materials; for silicon it is *h=0.7a* and for diamond slab it is *h=0.91a*. The diamond slab has the same optical thickness as the silicon slab. It will be shown in Section 3.2 that *h=0.91a* is the optimal thickness for a PCS with holes radius *R=0.29a*. The hole radius is varied between *R=0.2a* and *R=0.4a*. Figure 2 includes results for both silicon (grey) and diamond (black) PCSs. Note that the widths of the first gaps for the two materials are comparable for any size of the air holes. However, the gap centre of diamond occurs for higher frequencies than for silicon due to the smaller refractive index. Consequently, the in-plane quality factors $Q_{//}$ for the two materials are similar, whereas the out-of-plane quality factor $Q_{\perp}$, which relies on TIR, for diamond is expected to be smaller. For both materials, reducing the hole size lowers the central frequency of the gap and therefore the vertical confinement improves, increasing $Q_{\perp}$. But at the same time, the gaps become narrower and therefore $Q_{//}$ decreases and the modal volume increases. Therefore this in-plane mode delocalization contributes to higher $Q_{\perp}$, as pointed out in Ref. [25]. We can increase the number of periods and therefore increase $Q_{//}$, but the modal volume is essentially not affected by this. In choosing the hole size we therefore have a trade off: small (large) holes lead to large (small) Q, but also to large (small) modal volumes. Results presented in Fig. 2 indicate that there is a broad optimum for the holes size. Our choice of *R=0.29a* follows the most common choice.

3.2 Quality factors and modal volume

We consider a M1 cavity as described by Zhang *et al* in Ref. [7]. We use the same parameters, hole radius is *R=0.29a*, and the thickness of the slab is *h=0.7a* for silicon and a thicker slab, *h=0.91a*, is used for diamond. The cavity is surrounded by 11 periods in all directions. Increasing the number of periods to 14 changes the quality factor by less than 2%. This means that the total Q approaches $Q_{\perp}$. Numerical parameters for the calculations are presented in Table 1. At first we use a computational window of including the entire structure to find the resonances and their symmetries. Then the computational window is reduced eight times using the field symmetry properties. Satisfactory convergence is obtained by using 20 points per period when calculating quality factors up to a few thousand, and 32 points per period for higher quality factors. The perfectly-matched layer width and the height of the computational window are chosen to be quite large as they strongly affect convergence (see Table 1).

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Table 1. Numerical parameters in the calculations

N	x_{max}/a	y_{max}/a	z_{max}/a	$\Delta x/a$	$\Delta y/a$	$\Delta z/a$	w_x/a	w_y/a	w_z/a
32	15.50	1.82	15.00	0.030	0.030	0.027	2.00	2.00	1.73

N-number of points per period; x_{max}, y_{max}, and z_{max}- computational window size of 1/8 of the structure; Δx, Δy and Δz-grid size; w_x, w_y and w_z- perfectly matched layer width.

For both materials, FDTD simulations indicate that there is one distinct resonance peak within the lowest band gap of the un-optimized structure consisting of two degenerate dipole-like modes. As expected, the quality factor in diamond $Q_{dia}=144$ is smaller than the silicon value $Q_{Si}=400$. However, both values are too small to satisfy QIT requirements [19].

To optimize these cavities, we first vary the displacements of the left and right neighbouring air holes from $d=0.15a$ to $d=0.25a$. The optimum appears at $d=0.21a$, as for silicon [6 7]. One effect of shifting the holes in the x-direction is lifting the modes' degeneracy [5]. Another effect is that a new resonant mode appears near the upper PBG edge, $\tilde{\omega} = \omega a / 2\pi c$ =a/λ=0.400. The calculated quality factor for that mode is $Q=2600$. As this mode has a higher quality factor than the modes in the gap center, we further concentrate on it. We next reduce the holes radius above and below the cavity. Figure 3(a) shows the calculated quality factors as a function of the hole radii r that are varied between $r=R=0.29a$, when the holes are not modified, and $r=0.19a$. The displacement is fixed at $d=0.21a$. The maximum, $Q=3.0\times10^4$, appears at $r=0.22a$. With this second modification, the modes from the band edge are pulled down towards the middle of the upper half of the band gap [7]. The resonant frequency, $\tilde{\omega}$=0.389, has the same relative position within the band gap as in the silicon slab, but the diamond band gap is higher and therefore the quality factor is smaller.

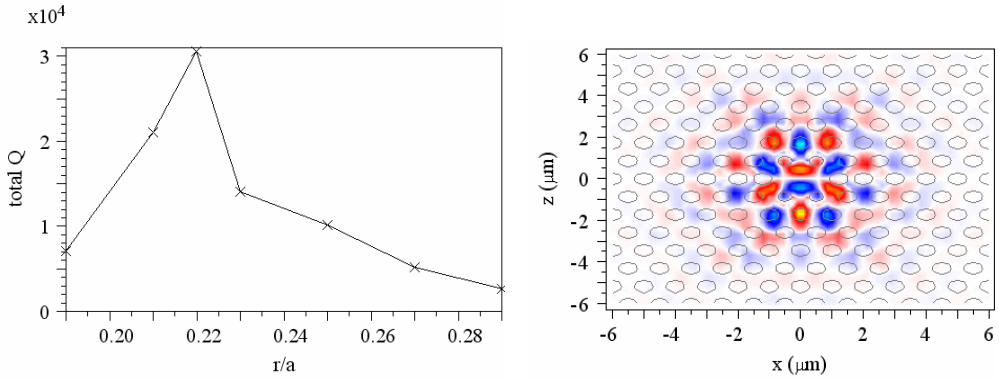

Fig. 3. (a) Quality factor of the diamond PCS as a function of radius of the holes above and below the cavity with fixed displacement d=0.21a; and (b) electric field amplitude E_x of the resonant mode in the center of the slab. The coordinate axes are defined in Fig. 1(a).

The major electric field component, E_x, at the centre of the diamond slab is shown in Fig. 3(b). It is symmetric in the x- and y-directions and anti-symmetric in the z-direction as for the corresponding mode of the silicon slab.

With these modifications Zhang *et al* reported a quality factor $Q=5.85\times10^5$ within a small modal volume using a silicon based PCS [7]. Having done a similar optimization for the diamond slab we obtain a quality factor $Q=3.0\times10^4$ within a modal volume of $V= 1.02\ (\lambda/n)^3$. The modal volume of the diamond slab is less than twice the modal volume of the equivalent mode in a silicon slab.

It is interesting to notice that the optimum occurs for both materials at the same parameters (displacement in the horizontal direction and radius of the neighbouring holes in the vertical direction). Varying the thickness of the diamond slab from $h=0.7$a to $h=1.1a$ we find that the optimum does appear at $h=0.91a$ for the given holes radius.

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We have also tried to apply other cavity optimization approaches that have already been applied to silicon PCSs [2, 6]. These methods do increase the quality factor for the diamond slab as well, but the best results were obtained for the modification presented above. For example, we considered the structures of Akahane *et al* in Ref [6], in which three holes are missing. Using the same parameters for the bulk PCS as before, and following the optimization procedure of Akahane *et al*, we obtained $Q=6000$, compared to $Q=1\times10^5$ for silicon [6]. This optimum appears for the same displacement as for silicon: the hole closest to the cavity is shifted by $d_1=0.21a$, the next one by $d_2=0.025a$ and the last one by $d_3=0.2a$.

4. Conclusion

We have compared the *Q*-values and modal volume that can be achieved in PCS made from silicon and from diamond, which has a somewhat lower refractive index. Using a number of different approaches to optimize these parameters, all originally developed for silicon PCS, we find that small modal volume microcavities can be designed in diamond PCS, with $Q=3.0\text{x}10^4$, smaller than in silicon. We believe that these results hold promise for future use of photonic crystal for quantum information purposes. Though this value is too small for full QIT experiments [19], it is sufficient for proof-of-principle demonstrations. Higher values of *Q* may possibly be achieved using PCS heterostructures [26].

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