Design of photonic crystal microcavities in diamond films

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Abstract: We design photonic crystal microcavities in diamond films for applications in quantum information. Optimization of the cavity design by “gentle confinement” yields a high quality factor $Q > 66000$ and small mode volume $V \approx 1.1 \left(\frac{\lambda}{n}\right)^3$. In view of experimental applications we consider the influence of material absorption on the cavity Q factors and present a simple interpretation in the framework of a one-dimensional cavity model.

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References and links

1. Introduction

Optically active defect centers (color centers) in diamond have attracted significant interest for applications in quantum information and quantum optics in recent years [1]. For single nitrogen-vacancy (NV) centers a number of key experiments have been demonstrated, e.g. single photon emission [2, 3], coherent oscillation of a single electron spin [4], two-qubit quantum...
gates [5] and coherent population trapping [6]. Among the many known color centers in diamond [7] there have been investigated only three centers at the single emitter level: NV centers, nickel-nitrogen (NE8) centers [8, 9, 10] and silicon vacancy (SiV) centers [11]. The latter two are of particular interest for the realization of optical quantum bits (qubits) due to their narrow line-widths of 1.2 nm [8] and < 5 nm [11], respectively, at room temperature. The term “optical qubit” here refers to the ability to optically initialize, manipulate and read-out the qubit state. In high-quality diamond and at cryogenic temperatures the phonon-broadened lines of all three centers approach linewidths limited by radiative lifetimes of approximately 10-20 ns [7].

There have been a number of recent proposals for employment of color centers in diamond as optical qubits in quantum networks [12], quantum gates [13], probabilistic quantum computers [14, 15] or for demonstrations of quantum phase transitions of light [16]. All of these proposals require the coupling of single defect centers to cavity modes with high quality factor \( Q \) and small mode volume \( V \), enabling the transfer of quantum information between internal electronic or spin states and photonic quantum bits. The emitter-cavity coupling can be further qualified depending on the application: the weak-coupling regime with \( g \ll (\gamma_\perp, \kappa) \) suffices e.g. for realizations of quantum networks whereas quantum gates and quantum phase transitions of light require a strong coupling \( g \gg (\gamma_\perp, \kappa) \), where \( g \) is the emitter-field coupling constant (vacuum Rabi frequency), \( \gamma_\perp \) is the emitter dipole decay rate and \( \kappa \) the cavity field decay rate. The figure of merit for the weak-coupling regime is the Purcell factor, i.e. the enhancement factor of the spontaneous emission rate, given by

\[
F = \frac{3Q}{4\pi^2} \frac{\left(\frac{\lambda}{n}\right)^3}{V}, \tag{1}
\]

where \( \lambda \) is the cavity mode wavelength and \( n \) the material refractive index. An optimization of the Purcell factor thus requires a maximum ratio \( Q/V \). The cavity decay rate is given by \( \kappa = \omega_c/(4\pi Q) \), with the cavity mode frequency \( \omega_c \), and the vacuum Rabi frequency is defined as \( g = \gamma_\perp \sqrt{V_0/V} \), with \( V_0 = c\lambda^2/(8\pi\gamma_\perp) \) [17]. The conditions \( g \gg \kappa \) and \( g \gg \gamma_\perp \) thus demand maximization of \( Q/\sqrt{V} \) and \( 1/\sqrt{V} \), respectively. With these equations we can estimate the boundary conditions for photonic crystal cavity design: At room temperature, the phonon-broadened emission lines allow for spontaneous emission enhancement due to cavity coupling if the cavity linewidth \( 2\kappa \) is larger than the emission bandwidth \( \Delta \nu \). For the NE8 center, \( \Delta \nu = 1.2 \text{ nm} \) (at \( \lambda \approx 800 \text{ nm} \)) puts an upper limit on the cavity quality factor \( Q < 670 \). However, as the mode volume of photonic crystal cavities can be extremely small, i.e. on the order of \( V \approx 1(\text{nm}/n)^3 \), we still obtain a Purcell factor of \( F \approx 50 \). On the other hand, strong emitter-cavity coupling might only be observed at low temperatures (\( \approx 4 \text{ K} \)) where lifetime-limited linewidths are attainable. To give an example, using the radiative lifetime of SiV centers, \( \tau = 19 \text{ ns} \) [18], resulting in \( \gamma_\perp = 2\pi \times 4.2 \text{ MHz} \), the conditions for strong coupling are (i) \( \sqrt{V} \ll \sqrt{V_0} = \sqrt{8.5 \times 10^3} \), where the volumes \( V \) and \( V_0 \) are given in units of \( (\lambda/n)^3 \), and (ii) \( Q \gg 2.65 \times 10^3 \sqrt{V} \). Condition (i) is easy to fulfill for a photonic crystal cavity. Taking again \( V \approx 1(\text{nm}/n)^3 \), (ii) reduces to \( Q > 2650 \), which is fairly reasonable as we show below. One should keep in mind, however, that the given values for \( g \) are valid for optimum coupling of the emitter to the absolute maximum of the cavity field only. Non-ideal placement of the emitter and fabrication tolerances of the photonic crystal structure both reduce the effective coupling. Technically, the realization of an atom-photon-interface requires technologies for positioning defect centers at predefined locations and creating photonic micro-structures in diamond [19]. Investigations of microcavities in diamond so far did not extend beyond few theoretical simulations of designs of photonic crystal microcavities [20, 21] and first experimental demonstrations of cavity modes in diamond microdisk resonators [22] and photonic crystal defect cavities [23].

As shown above, photonic crystal microcavities are well suited for applications in quantum
information as they offer high quality factors $Q$ and small mode volumes $V$ together with the possibility of scalable architectures. Recent investigations of microcavities in two-dimensional photonic crystal slab structures in diamond have yielded theoretical $Q$ factors of up to $7 \times 10^4$ [21], sufficient for proof-of-principle demonstrations of emitter-cavity-coupling. We here extend first investigations on diamond photonic crystal defect cavity design [20] in two ways: First, we show that by optimizing the defect cavity design of [20] according to the principles of “gentle confinement” [24, 25] the $Q$ factor can be further increased. Second, for practical realizations of photonic crystals in diamond one has to take into account the material absorption. For creating two-dimensional slab structures, thin diamond films are required as base material, e.g. nano-crystalline chemical vapor deposition (CVD) diamond. CVD diamond films, however, show strong absorption in the spectral range of color center emission [26] due to the presence of $sp^2$-bonded carbon. We here show the influence of material absorption on the cavity $Q$ factors and present a simple interpretation in the framework of a one-dimensional cavity model.

2. Cavity design

The photonic crystal (PhC) structures consist of a thin free-standing diamond membrane (slab) with a periodic array of circular air holes. Confinement of light is realized by distributed Bragg reflection in the plane of periodicity ($xy$) and by total internal reflection in the perpendicular plane ($z$). Microcavities are formed by point or line defects in the air hole lattice. Analogous PhC slab structures have been successfully employed in semiconductor quantum optics yielding strong coupling of single semiconductor quantum dots [27, 28]. For diamond, however, the crucial parameter is the relatively low refractive index of $n = 2.4$ [7], leading to smaller PhC bandgaps and weaker mode localization. It is thus important to investigate whether one can still realize small mode volume high-$Q$ cavities.

2.1. Lattice type

For the design of the PhC microcavity we follow a step-by-step approach, starting with the fundamental lattice type of the PhC slab structure. The most common choices for the basic lattice type are square or triangular arrays of air holes in a dielectric slab. Figure 1 shows the frequencies of the upper and lower edge of the first (fundamental) band gap for TE-modes in diamond PhC slab structures with infinite extension in $z$-direction as function of the air hole radius $R$ in units of the lattice constant $a$. The PhC band diagrams were calculated using a plane wave expansion method [29].

The basic criteria for the choice of lattice type and air hole radius $R$ are as follows: a wide band gap supports confinement of modes in the plane of the PhC ($xy$). For finite height slab structures as discussed in the next section, low mid gap frequencies allow for good confinement in vertical direction as a larger fraction of the mode’s $k$-space components lies below the light line [30](see also discussion and definition of light line in Sec. 2.2). According to these criteria, a square lattice structure is obviously a bad choice for diamond PhC as the relative frequency width $\Delta \omega / \omega_{\text{midgap}}$ of the band gap is only 2.6% and mid gap frequencies are very high. A triangular lattice, on the other hand, offers a relative gap width of 30% at a mid gap frequency of $\omega_{\text{midgap}} / (2\pi c/a) \approx 0.4$ for an optimum air hole radius $R = 0.4 a$.

2.2. PhC slab

The next step in PhC microcavity design is consideration of a finite height slab structure while keeping the basic lattice fixed. Figure 2 shows the first 4 even (TE-like) bands of a diamond slab with height $h$ suspended in air and patterned with a triangular array of air holes with radius $R$. 

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Here, the frequencies of the band gap edges are determined by the maximum of the first TE-like-band and the minimum of the second TE-like-band, as well as by the intersections of the bands with the light line. For a given air hole radius $R$, the slab height $h$ determines the properties of the photonic band gap: for increasing $h$ the mid-gap frequency monotonically decreases which allows for better vertical confinement. On the other hand, there exists an optimum for the band gap width. Very thin slabs exhibit band gaps at high frequencies where the mode spacing is small, very thick slabs pull down additional modes below the light line, i.e. they are no longer single-mode waveguides. Both effects lead to a decrease of the band gap width. For
$R = 0.4\ a$ we find the largest band gap for an optimum slab thickness of $h = 0.75\ a$ as displayed in Fig. 2(a).

Based on this simple approach of maximizing the photonic band gap, optimum mode confinement and thus maximum $Q$ factors would be expected for cavity modes lying close to the mid gap frequency of the optimized band gap. Figure 2(a) shows the mode frequency of a M1 cavity (see Sec. 2.3) in the optimized slab structure ($R = 0.4\ a, h = 0.75\ a$) which indeed lies close to mid-gap. However, the calculated quality factor of this mode is just $Q \approx 500$. For comparison, Fig. 2(b) displays band gap and mode frequency of a PhC defect cavity with slab parameters which are derived from a systematic optimization of the cavity $Q$ factor ($R = 0.29\ a$ and $h = 0.91\ a$, see Sec. 2.4). Despite a smaller band gap width and the fact that the mode frequency lies close to the upper band gap edge, this cavity mode exhibits $Q$ factors in excess of 60000. Part of this effect stems from the lower mid-gap frequency and the larger fraction of the mode wavevectors below the light line. The major part of the $Q$ factor increase, however, is due to a reduction of radiation losses of guided modes following the principle of “gentle confinement” [24] which is elaborated in the next section.

### 2.3. M1 cavity

As a next step in the design of diamond PhC microcavities we have to lay out the defect cavity design. As we wish to yield high $Q$ cavities with small mode volume $V$ we choose a cavity design based on a single defect, i.e. one missing air hole. We here adopt the design of Refs. [31, 20], coined “one missing hole waveguide-section cavity (M1)**, as a starting point for further optimization. Alternatively, one could consider a double-heterostructure type cavity as discussed in [21]. Such cavities feature very high theoretical quality factors up to of $Q = 2.4 \times 10^7$ in silicon at the expense of slightly higher mode volumes [32]. However, first investigations of double-heterostructure cavities in diamond [21] indicate that the $Q$-factors are limited to $Q \approx 7 \times 10^4$ and further improvement seems difficult as the cavity mode lies very close to the band edge. As the mode volume of double-heterostructure type cavities in diamond is about twice as large as for M1 type cavities, but $Q$-factors turn out to be almost identical, we adhere to the M1 design.

The basic goal of cavity design optimization should be to increase the quality factor $Q$ without delocalizing the mode, i.e. increasing the mode volume $V$. The quality factor $Q$ can be separated into $1/Q = 1/Q_{\parallel} + 1/Q_{\perp}$ [31, 33], where the in-plane quality factor $Q_{\parallel}$ describes the confinement due to distributed Bragg reflection in the $xy$-plane, and $Q_{\perp}$ refers to the out-of-plane loss due to mode $k$-space components not matching the conditions for total internal reflection (TIR) at the slab boundaries. In theory, ideal in-plane confinement (large $Q_{\parallel}$) can be achieved by increasing the number of air hole layers surrounding the cavity. Out-of-plane (vertical) radiation losses, on the other hand, appear if the mode wavevectors have vertical components $|k_{\perp}| \geq 0$, or equivalently, in-plane components $|k_{\parallel}| \leq k_0 = 2\pi/\lambda_0$, where $\lambda_0$ is the mode wavelength in air [24]. The condition $|k_{\parallel}| = k_0$ defines the “light line”, corresponding to the dispersion relation of light in air, whereas all wave vectors with $|k_{\parallel}| < k_0$ define the “light cone” of radiating modes. Fourier-space analysis of the cavity field distribution reveals that a gentle variation of the mode field envelope function suppresses vertical radiation losses where the ideal envelope is a Gaussian function [24, 33]. This gentle variation of the field envelope is achieved by modifying the geometry of the next-neighbor lattice points surrounding the single defect [31, 34]. Figure 3 shows the geometry of the defect cavity and the next-neighbor lattice points together with the nomenclature used.

In detail, we displace the two next-neighboring holes (B) in $x$-direction by a distance $d$ and change their radius from $R$ to $R_B$. The four next-neighboring holes in $\Gamma - K$ direction (C) are displaced along the lattice vector by a distance $m$; their radius is modified to $R_C$. Finally, we
vary the radius $R_D$ of the four second-next neighbor holes (D).

### 2.4. Optimization of quality factor

For the calculation of the cavity mode field distribution and quality factor we use a finite difference time domain (FDTD) method [35]. The simulated PhC structure is a $20a \times 20a$ super cell with height $8a$, surrounded by perfectly matching layers as absorbing boundaries. We use a resolution of 16 points per lattice period. For each simulation we start with excitation of the PhC structure with a broadband source to find resonant modes and symmetries of field distributions. For calculating mode $Q$ factors we then make use of the mode symmetries and employ a narrow-band source. Resonant mode frequencies and decay rates are extracted by a filter diagonalization method [35]. The mode volume $V$ is calculated by [17]:

$$ V = \frac{\int \int \int |\vec{e}(\vec{r})| |\vec{E}(\vec{r})|^2 d^3\vec{r}}{\max |\vec{e}(\vec{r})| |\vec{E}(\vec{r})|^2}. $$

(2)

Out-of-plane losses caused by radiation perpendicular to the slab can be determined by a Fourier analysis of the in-plane field distributions $E_x, E_y, H_x, H_y$ in the air layer at a small distance ($\Delta z = \lambda/4$) above the slab surface [36]. The radiated power $P$ is proportional to:

$$ P \propto \int \int I \, dk_x dk_y \text{ with } I = \left| FT_2(H_y) + \frac{1}{\eta} FT_2(E_x) \right|^2 + \left| FT_2(H_x) - \frac{1}{\eta} FT_2(E_y) \right|^2 $$

(3)

where the integral runs over $k$-vectors inside the light cone, $\eta = \sqrt{\mu_0/\varepsilon_0}$, and $FT_2$ denotes the 2D Fourier transform. For all steps of the cavity design optimization, confinement and radiation losses of the cavity mode can be evaluated by calculating the fraction of Fourier components contained within the light cone.

As a starting point for the cavity optimization we adopt parameter values for the PhC structure from [20], listed in Tab. 1. For these parameters we find a high $Q$ cavity mode at $\omega_c = 0.384(2\pi c/a)$ with $Q \approx 27000$ and mode volume $V = 1.23(\lambda/n)^3$, close to the results of Ref. [20].
We now investigate the dependence of the cavity quality factor on each parameter to yield the optimum design. To this end we use an iterative procedure as the optimum value of each parameter critically depends on the choice of the other parameters.

We start out with the radius $R$ of air holes of the regular lattice. The optimum value $R = 0.29 \, a$ has been found in [20, 21] for slab heights of $h = 0.91 \, a$ and $h = 0.75 \, a$, respectively, and seems to be independent of $h$. We verify this choice of $R$ by calculating $Q$ vs. $R$ for yet a different slab height of $h = 0.77 \, a$ and find again an optimum for $R = 0.29 \, a$. Thus we keep $R = 0.29 \, a$ for the remainder of the paper.

The next variations of parameters of Set I were slight changes of the radii $R_B$ and $R_C$ of the next-neighbor holes $B$ and $C$. Keeping all other parameters constant we find a maximum $Q = 60420$ and $V = 1.15(\lambda/\pi a)^3$ for $R_B = 0.27 \, a$ and $R_C = 0.23 \, a$, arriving at a second set of parameters (see Tab. 2). These small variations of $R_B$ and $R_C$ already more than double the $Q$-factor found in first investigations [20].

As a next optimization step we check the choice of $h = 0.91 \, a$ [20] as optimum slab height. By varying $h$ within the interval $h = [0.85 \, a, 0.96 \, a]$ we find another increase in $Q$ from $Q = 60420$ for $h = 0.91 \, a$ to $Q = 62700$ for $h = 0.93 \, a$. The relative mode volume $V = 1.15(\lambda/\pi a)^3$ does not increase for the thicker slab as the mode frequency decreases at the same time. Thus we here adopt $h = 0.93 \, a$ as optimum slab height.

Finally we fine tune the cavity quality factor by again slightly varying next-neighbor hole radii $R_B$ and $R_C$, now together with the displacements $d$ and $m$ of the respective air holes, yielding a gentle confinement of the cavity mode. Figure 4 shows the quality factor $Q$ of the M1 cavity for variations of the parameters $R_B, R_C, d$ and $m$.

A slight reduction of both the shift $d$ and the radius $R_B$ of holes $B$ leads to higher quality factors whereas further variations of hole $C$ parameters just degrades $Q$. We find a maximum quality factor $Q = 66300$ with a small mode volume $V = 1.11(\lambda/\pi a)^3$ at frequency $\omega_c = 0.38212 \frac{2\pi c}{\lambda a}$ for the values of parameters given in Tab. 3. An additional variation of the radii $R_D$ of second next-neighbor holes $D$ within the range $R_D = [0.27 \, a, 0.31 \, a]$ does not further improve $Q$ but rather leads to smaller quality factors.

<table>
<thead>
<tr>
<th>$R$</th>
<th>$h$</th>
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<td>0.29</td>
<td>0.93</td>
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Figure 4 clearly shows that $Q$ very critically depends on very small variations of next-neighbor hole radii and displacements. This critical dependence makes fabrication of high qual-
Fig. 4. Quality factor $Q$ of the M1 cavity for variations of the next-neighbor hole dimensions and displacements. (a) $Q$ vs. $R_B$ and $d$. Other parameters are: $R = 0.29\,a$, $h = 0.93\,a$, $m = 0$, $R_C = 0.23\,a$, $R_D = 0.29\,a$. (b) $Q$ vs. $R_C$ and $m$. Other parameters are: $R = 0.29\,a$, $h = 0.93\,a$, $d = 0.19\,a$, $R_B = 0.25\,a$, $R_D = 0.29\,a$.

The amplitudes of electric and magnetic field components, $E_x$ and $H_z$, respectively, at the center of the slab ($z = 0$ plane) are shown in Fig. 5, revealing the confinement of the mode within the defect cavity.

Fig. 5. (a) Electric field ($E_x$) amplitude and (b) magnetic field ($H_z$) amplitude of the optimized M1 cavity resonant mode in the center plane of the slab ($z = 0$). Color scale: grey: diamond, white: air, blue and red: positive and negative field amplitudes, respectively.

Fig. 6 displays the $k$-space intensity $I$ defined by eq. (3) for the optimized M1 cavity (a) and a non-optimized cavity with $Q \approx 25000$ (b).

The comparison of optimized and non-optimized cavity mode $k$-space intensity distribution reveals the effect of gentle confinement: for the optimized cavity mode the intensity within the leaky region (light cone) is greatly reduced and the high-intensity components lie farther away from the light cone as required for a high-$Q$ cavity mode [33].
Fig. 6. $k$-space intensity distribution $I$ for resonant mode of (a) optimized M1 cavity (parameter set III) and (b) non-optimized M1 cavity (parameters: $R = 0.28\, a$, $h = 0.77\, a$, $d = 0.21\, a$, $R_g = 0.28\, a$, $m = 0$, $R_C = 0.22\, a$, $R_D = 0.28\, a$, $Q \approx 25000$). The white circle shows the light cone boundary $k_\parallel \leq k_0$.

3. Absorption losses

Most investigations of photonic crystal microcavities assume ideal, lossless materials. However, for practical realizations of photonic crystals one has to take into account realistic parameters, in particular material absorption. This is especially important for thin diamond films which are required to create two-dimensional slab structures. Chemical vapor deposition (CVD) diamond films usually show strong absorption in the spectral range of NV, SiV and NE8 color center emission ($\approx 630 - 800\, \text{nm}$) [26] due to the presence of $sp^2$-bonded carbon. As the absorption is due to sub-gap electronic transitions it only changes very weakly with temperature and does not vanish at cryogenic temperatures. The absorption strength critically depends on the diamond grain size and is generally highest for nano-crystalline CVD diamond (grain sizes $< 10\, \text{nm}$) and smallest for poly-crystalline CVD diamond (grain sizes $> 100\, \text{nm}$) and single-crystal diamond films. With increasing grain sizes, however, optical scattering losses become more prominent. Single-crystal diamond films exhibit the best overall optical properties but are very difficult to process into membrane structures required for photonic crystal slabs [19]. We thus focus our discussions on nano-crystalline CVD diamond films.

We take into account material absorption by defining a model dielectric function for the FDTD simulations where we artificially introduce a dielectric resonance close to the cavity mode frequency $\omega_c$:

$$
\varepsilon(\omega, \vec{r}) = \varepsilon_\infty(\vec{r}) + \frac{\omega_c^2 \Delta \varepsilon}{\omega_c^2 - \omega^2 - i \omega \gamma}
$$

Here $\varepsilon(\omega, \vec{r})$ denotes the material dielectric constant, $\varepsilon_\infty$ the background dielectric constant for $\omega \to \infty$, $\gamma$ and $\Delta \varepsilon$ the width (FWHM) and amplitude of the dielectric resonance, respectively. In the limit of weakly absorbing media, i.e. $\varepsilon_i \ll \varepsilon_r$, with the real and imaginary part of the dielectric constant, $\varepsilon_r$ and $\varepsilon_i$, respectively, the absorption coefficient $\alpha$ is calculated as:

$$
\alpha(\omega) = -\frac{k_0}{n} \frac{\omega_c^2 \Delta \varepsilon \omega \gamma}{\omega_c^2 - \omega^2 - i \omega \gamma}^2
$$

The limit of weakly absorbing media is a good approximation for diamond as the maximum measured absorption coefficient of bad quality diamond films is $\alpha \approx 10^4\, \text{cm}^{-1}$ at the SiV absorption peak.
center wavelength of 740 nm, which still yields $\varepsilon_i = 0.283 \ll \varepsilon_r = 5.76$. Fig. 7 shows real and imaginary part of an example dielectric function.

Fig. 7. Real and imaginary part of model dielectric function used to introduce material absorption into FDTD calculations. Parameters (see eq. (4)) are: $\varepsilon_\infty = 5.76$, $\omega_c = 0.384$, $\gamma = 0.4$, $\Delta \varepsilon = 0.005$. The dashed red line shows the frequency of the resonant cavity mode, the solid red curve the Gaussian frequency distribution of the source used to excite the cavity mode in the FDTD calculations.

Amplitude and width of the dielectric resonance are tailored to yield a certain absorption coefficient $\alpha$ at the cavity mode frequency while at the same time keeping the change $\Delta \varepsilon_r$ of the real part of the dielectric function to a minimum. To this end we generally choose a large value of $\gamma$ together with a small $\Delta \varepsilon$. To give an example we use the M1 cavity parameter set II yielding $Q = 60420$ at $\omega_c = 0.384$. For the choice of parameters in Fig. 7, i.e. $\varepsilon_\infty = 5.76$, $\gamma = 0.4$, $\Delta \varepsilon = 0.005$ and an emission wavelength of $\lambda_0 \approx 740$ nm for the SiV center, we get an absorption coefficient of $\alpha = 170 \text{ cm}^{-1}$ at the cavity mode frequency $\omega_c$. The real part of the dielectric function at $\omega_c$ remains at the background value $\varepsilon_r(\omega_c) = \varepsilon_\infty = 5.76$ as desired. However, we have to examine the consequences of the variation of $\varepsilon_r$ in the vicinity of the cavity mode frequency. For this purpose, we consider the frequency interval $\Delta \omega_S = 0.02(2\pi c/a)$ around $\omega_c$ covered by the source used to excite the cavity mode in the FDTD calculations (see Fig. 7). Within the interval $[\omega_c - \Delta \omega_S/2, \omega_c + \Delta \omega_S/2]$, $\varepsilon_r(\omega)$ only changes by $\delta \varepsilon_r = 0.006$, i.e. the relative variation $\delta \varepsilon_r/\varepsilon_r(\omega_c) \approx 10^{-3}$. We now calculate the cavity $Q$-factors using a constant set of geometry parameters (parameter set II), but taking into account the different values of the dielectric constant’s real part $\varepsilon_r(\omega)$ introduced by the dielectric resonance in the frequency interval of the FDTD excitation source. The deviation of $Q$-factors due to the variations of $\varepsilon_r(\omega)$, $\Delta Q = \max |Q(\varepsilon_r(\omega_c)) - Q(\varepsilon_r(\omega_c \pm \Delta \omega_S/2))|$, is very small: $\Delta Q = 20$ or $\Delta Q/Q = 3.3 \times 10^{-4}$. By inspection of various parameter combinations for the dielectric function of eq. (4) we find an upper boundary for $\Delta Q/Q < 2 \times 10^{-3}$. Thus, to a very good approximation, we have artificially introduced absorption losses or an imaginary dielectric constant into the FDTD calculations without affecting the real part of the dielectric constant.

We now use the dielectric function defined above to calculate cavity $Q$-factors for a lossy material, using the M1 cavity design as given by parameter set II. Fig. 8 shows the calculated quality factor $Q$ as function of the absorption coefficient $\alpha$. 

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The strong decrease of $Q$ with increasing absorption losses displayed in Fig. 8 fundamentally alters predictions for photonic crystal microcavities in diamond. For ultra-nanocrystalline diamond films of high quality we measure absorption coefficients of $\approx 150 \pm 20$ cm$^{-1}$ at the SiV center emission wavelength of 740 nm, yielding a reduction of the predicted quality factor from $Q_0 = 60422$ to $Q_{\text{real}} \approx 1350$. We arrive at about the same value of the realistic $Q$-factor $Q_{\text{real}}$ for the optimized M1 cavity (parameter set III) with $Q_0 = 66300$ as the quality factor again mainly is determined by absorption losses. This strong dependence of $Q$-factors on material absorption might be the major reason besides scattering losses for low $Q$-factors experimentally observed so far in diamond photonic crystal cavities [23].

For the dependence of $Q$ on $\alpha$ we find a simple law following [37, 38, 39]. First, we note that the cavity $Q$-factor in presence of material losses can be decomposed into:

$$\frac{1}{Q} = \frac{1}{Q_0} + \frac{1}{Q_{\text{abs}}}$$

where $Q_0$ is the cavity $Q$-factor for an ideal, lossless material and $Q_{\text{abs}}$ denotes a quality factor due to absorption losses. In order to define $Q_{\text{abs}}$ we remember the definition of the quality factor $Q$ by the decay of the intracavity photon number $\phi(t)$, with

$$\phi(t) = \exp(-t/\tau_c)\phi(0) \equiv \exp(-\omega t/Q)\phi(0).$$

Here $\tau_c = 1/\Delta \omega_c$ denotes the photon lifetime in the cavity mode and $\Delta \omega_c$ the cavity bandwidth. From these equations one derives the usual expression for the quality factor: $Q = \omega \tau_c = \omega / \Delta \omega_c$. The “absorption $Q$-factor” $Q_{\text{abs}}$ is defined analogously to eq. (7) by the decay of the intracavity photon number due to absorption: $\phi_{\text{abs}}(t) = \exp(-t/\tau_{\text{abs}})\phi(0)$, introducing $\tau_{\text{abs}}$ as average time after which a photon is removed from the cavity mode by absorption. $\tau_{\text{abs}}$, on the other hand, can be expressed by the usual absorption length $L_{\text{abs}} = \alpha^{-1}$ as $\tau_{\text{abs}} = L_{\text{abs}}/c_m = 1/(\alpha c_m)$, where $c_m$ is the phase velocity in the material. In a simplified approach we substitute $c_m$ using a linear dispersion relation $\omega = c_m k$ and arrive at:

$$\phi_{\text{abs}}(t) = \exp(-\omega t/k)\phi(0) \equiv \exp(-\omega t/Q_{\text{abs}})\phi(0).$$
From eq. (8) and the relations $k = 2\pi n_r/\lambda$ and $\alpha = 4\pi n_i/\lambda$ (for weakly absorbing media), where $n_r$ and $n_i$ are real and imaginary part of the material refractive index, respectively, we obtain a definition for $Q_{\text{abs}}$ (cf. [39]):

$$Q_{\text{abs}} = \frac{k}{\alpha} = \frac{n_r}{2n_i}. \tag{9}$$

The usage of the linear absorption coefficient in eqs. (8,9) means that a photonic crystal microcavity which obeys eq. (6) is formally equivalent to a simple one-dimensional cavity where the absorption losses are distributed over the cavity length. The solid line in Fig. 8 shows the simple law of eqs. (6,9) without any fit parameters. The agreement of $Q$ factors derived from eq. (6) and the $Q$-factors calculated from FDTD simulations including material losses is very well. Thus, the simple equation (6) allows for easy prediction of cavity quality factors in the presence of absorption. From the simulation of a single photonic crystal cavity and the use of a linear dispersion relation it is not clear, however, whether eq. (6) holds as a general law and whether its predictions are valid for a larger range of cavities. This question is subject of current investigations.

4. Conclusion

We have investigated photonic crystal defect cavities in thin diamond films, demonstrating that by employing the principles of gentle confinement cavity $Q$-factors can be improved over previous designs. Our calculations for an optimized cavity design yield maximum $Q$-factors of 66300 with a mode volume $V = 1.1(\lambda/n)^3$. Due to these high quality factors $Q$ and small mode volumes $V$ together with the possibility of scalable architectures, photonic crystal microcavities are well suited for applications in quantum information.

In addition, we have taken into account realistic material parameters for the FDTD simulation of photonic crystals, i.e. absorption of nano-crystalline diamond films in the wavelength range of color center emission. We have calculated the influence of material absorption on the cavity $Q$-factors and find a strong decrease of $Q$ with increasing absorption coefficient. We also demonstrated that the prediction of $Q$-factors in the presence of losses is greatly simplified by a one-dimensional cavity model.

Taking into account absorption losses in diamond films, quality factor $Q$ and Purcell factor $F$ for the optimized cavity reduce to $Q \approx 1350$ and $F \approx 92$. Thus, even for a lossy material demonstrations of modified spontaneous emission and emitter-cavity coupling at room-temperature should be feasible. For applications in quantum information processing demanding strong emitter-cavity coupling, however, our estimations show that for the coupling of SiV centers at cryogenic temperatures a minimum quality factor $Q > 2800$ is required. As this limit is only a factor of two higher than our calculated results, a realistic solution to this problem could be further work on improvement of purity of nano-crystalline diamond films or the use of single-crystal diamond exhibiting much better optical properties.

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