Numerical study of exact Purcell factors in finite-size planar photonic crystal waveguides

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The waveguide-length sensitivity on modified spontaneous emission in finite-size planar photonic crystal (PC) waveguides is investigated by numerically computing the exact Purcell (enhanced emission) factor. An unusual dependence on the number of waveguide unit cells and on the waveguide facet truncation is found, allowing one to nanoengineer large Purcell factors in excess of several hundred. Besides having important applications for single-photon sources, these results offer physical insight into the nature of light–matter interactions in miniaturized finite-size PC waveguides, where periodic Bloch-wave analysis breaks down.

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The understanding of modified spontaneous emission (SE) is important for fundamental science and for applications in quantum information science. In 1949, Purcell pointed out that when an emitter is embedded inside a closed resonant cavity, there can be a significant enhancement in the SE rates [1] owing to the increase in the local density of photon states (LDOS), a phenomenon called the the Purcell effect. For an open cavity system, Kleppner [2] showed that the SE rates can also be enhanced using a cylindrical wire waveguide with an emission frequency lying near the waveguide-mode edge, which originates from low group velocity propagation modes; one of the possible advantages of the open waveguide is that it also supports efficient channeling and extraction of light.

Recent years have seen a surge of research activity related to the control and manipulation of SE rates in nanoscale semiconductors. The SE rates from a single-photon emitter, e.g., an artificial atom or a single quantum dot (QD), are strongly affected by the LDOS of the surrounding environment. In particular, planar photonic crystals (PCs) are an attractive platform for controlling the emission from single QDs, and several pioneering experiments have now probed the strong coupling regime using a single electron-hole pair [3,4]. Less well studied is the modified SE rate from QDs embedded in open system PC waveguides [5], which has several advantages over the closed PC cavity structures. For example, PC waveguides enable broadband enhanced β factors and support rate enhancements for slow light modes. Viasnoff-Schwoob *et al.* [6] achieved a modest enhancement in the emission rates of a QD embedded in the PC wires by coupling to leaky modes above the light line. Manga Rao and Hughes [7] and Lecamp *et al.* [8] investigated SE rate enhancements and collection efficiency from a single QD in an infinitely long PC waveguide, reporting Purcell factors >25 and β factors >0.85. However, long waveguides are now known to have extrinsic scattering problems associated with unavoidable fabrication imperfections [9], and they do not easily support the positioning of single QDs.

We have recently proposed a single-photon device that exploits a short finite-length PC waveguide [10], demonstrating large emission factors of >150 in a 20 unit-cell long waveguide. Using such short length waveguides, a photon gun can be engineered by surrounding the waveguide with air on both sides or by also using a PC mirror on one side of the waveguide (acting as a reflector). Unfortunately, no investigation into the unknown role of unit-cell number and facet interface truncation was studied. In this Letter, we present a rigorous systematic study of enhanced SE in finite-size PC waveguides as a function of the unit-cell number. The truncation of the ends of the finite-size PC waveguides (facets) with either half a unit cell less, or half a unit cell more, is investigated and found to have a significant influence on the LDOS and SE factors. Figure 1(a) shows a schematic of the finite-size PC waveguide formed from a short

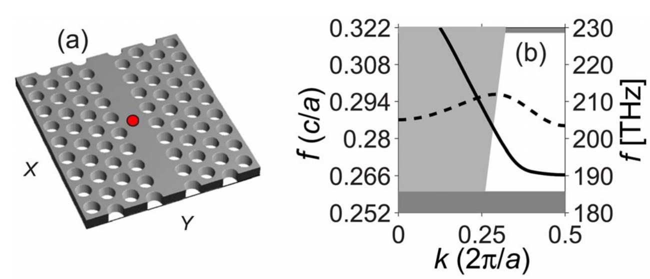

Fig. 1. (Color online) (a) Dielectric profile of a finite-size planar PC waveguide (W1), where propagation is along the x axis and a single QD (filled circle) is embedded near the center of the slab. The propagation mode is bound by total internal reflection in the z direction by the slab. The structure parameters used in the simulations are as follows: hole radius $r=0.275a$, slab thickness $0.5a$, refractive index $n=\sqrt{12}$, and lattice constant $a=420$ nm. (b) Band structure of modes (solid and dashed curves) corresponding to an infinite-length planar PC waveguide shown within the TE-like bandgap [parameters as in (a)]. The gray shaded region above the light line represents the continuum of radiation modes.

section of a regular infinite-length PC waveguide in which the usual Bloch mode analysis is employed. The single QD of interest is presumed to be embedded near the center of the waveguide/slab at a field antinode. The ideal band structure for an infinite-length PC waveguide is displayed in Fig. 1(b).

The photon emission rates are calculated by numerically calculating the exact photon Green function of the finite-size structure. The Green function is obtained from a polarization dipole solution of the three-dimensional (3D) Maxwell equations, using finite-difference time domain (FDTD) techniques [11], whereby the electric-field Green function, $\mathbf{G}(\mathbf{r},\mathbf{r}';\omega)$, describes the field response at $\mathbf{r}'$ to an oscillating polarization dipole at $\mathbf{r}$ as a function of frequency. In the weak coupling regime of interest, the normalized SE factor ($\equiv\mathbf{F}$) at the QD position ($\mathbf{r}_d$) is determined through

$$\mathbf{F}(\mathbf{r}_d,\omega)=\frac{\mathbf{d}\cdot\mathrm{Im}[\mathbf{G}^{\mathrm{PC}}(\mathbf{r}_d,\mathbf{r}_d;\omega)]\cdot\mathbf{d}}{\mathbf{d}\cdot\mathrm{Im}[\mathbf{G}^{\mathrm{hom}}(\omega)]\cdot\mathbf{d}}, \tag{1}$$

where $\mathbf{d}$ is a dipole moment of the QD electron-hole pair, $\mathrm{Im}[\mathbf{G}_{ii}^{\mathrm{hom}}]$, $(ii=xx,yy,zz)$ corresponds to that of the homogeneous bulk material with refractive index $n=\sqrt{\varepsilon}$, and $\mathbf{G}^{\mathrm{PC}}$ is the Green function of the complete PC under investigation. We employ the dipole approximation (QDs are much smaller than a wavelength) and assume that the QD dipole is located at the field maximum (unless stated otherwise), aligned with the polarization direction of the electric field. The expression above is an exact Purcell factor, in the sense that it accounts for coupling to all modes in the system without recourse to computing effective mode volumes and quality factors. For the mode of interest, we will consider $\mathbf{d}=d\mathbf{n}_y$ ($\mathbf{n}_y$ is a unit vector along y) and thus desire F_y, which is the enhanced emission rate that depends upon G_{yy}^{PC} and thus E_y.

We first study the behavior in the SE factors as a function of frequency by comparing the results for a few selected waveguide lengths, namely, 5, 10, 15, and 20 unit cells in the waveguide (x) direction surrounded by an air medium on either end of the waveguide. The peak emission factors occur at the resonance frequencies of 192.22, 190.98, 190.8, and 190.75 THz, with the longer guide producing the largest Purcell factor and the lowest frequency [nearer to the mode edge of infinite waveguide shown with the vertical dotted line in Fig. 2(a)]. Increasing the number of constituent unit cells in a waveguide causes the spectral peaks to asymptotically converge toward the mode edge and maximizes the emission factors. This phenomenon is a manifestation of the expected divergence in the LDOS near the mode edge for idealized infinite one-dimensional (1D) like waveguides (as the group velocity approaches zero); however, these longer waveguides suffer from extrinsic scattering owing to fabrication disorder [9], and the real LDOS becomes broadened as mentioned earlier. In contrast, since the LDOS enhancement for a finite-size structure is naturally broadened the overall effect of disorder on the proposed structures has a negligible influence on the LDOS and effective quality factors. The main effect is merely a possible disorder-induced resonance shift of the LDOS peak similar to the planar PC nanocavities [12]. In Fig. 2(b) we show a comparable PC waveguide that now has five layers of regular PC attached to one end of the waveguide; the regular PC section acts as an efficient broadband mirror and functions well even with just five layers of PC [10]. As can be recognized, a similar behavior arises as in the previous case, but now the SE factors are enhanced even further and the resonance peaks are pushed further away from the expected mode edge owing to the presence of a PC reflector. We also note from Figs. 2(a) and 2(b) that there exist small additional spectral peaks (cf. longer waveguide Purell factors) to the right of the main peak that are due to Fabry–Perot resonances; these peaks are specific to finite-size waveguides.

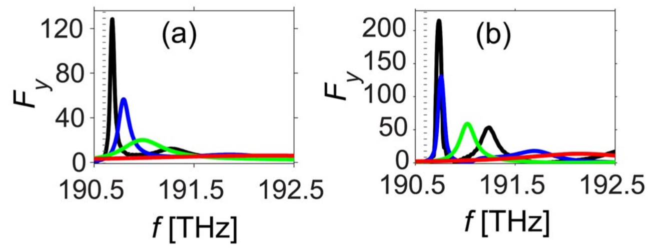

Fig. 2. (Color online) Enhanced SE (Purcell) factors as a function of frequency (relative to a homogeneous medium) for four different unit-cell numbers in a finite-size PC waveguide: 5, 10, 15, and 20 (with the longer waveguides producing the largest Purcell factors and the narrower peaks). (a) Surrounded by air on either side. (b) As in (a) but with one side of the waveguide surrounded by five layers of regular PC acting as a mirror [see also Fig. 3(b)].

Figure 3(a) shows the peak SE rates for a PC waveguide surrounded by air on both sides for a number of waveguide lengths ranging from 2 to 20 periods. Note that we have two cases based on the precise truncation of the waveguide ends (facets): (case i) truncation across the center of the nearest airholes on either side of the line-defect (filled boxes) and (case ii) truncation in between the nearest airholes (filled circles). In either case, the lengths of the waveguide scale with the integer number of lattice periods. The emission factors in both cases remain similar for shorter-sized waveguides (waveguide unit cells <8), but their values significantly differ as the length of the waveguide become larger. For example, the maximum emission factors for 20 unit cells are 128 and 165, respectively; this difference is attributed to a relative π-phase change ($\Delta\phi=ka/2\approx\pi$) in the propagating electromagnetic field from the QD (causing constructive or destructive interference). In Fig. 3(b) we show the maximum SE factors achievable by increasing the length of a finite PC waveguide on one end by half a unit cell while the other end is surrounded by five layers of a regular PC (mirror). Again, we have two cases based on the truncation of the waveguide section with labels the same as before. The SE factors for 19.5 and 20 unit cells are 252 and 205, respectively.

In both of these modeled structures we note that the waveguide truncation in between the nearest waveguide airholes leads to greater enhancement of

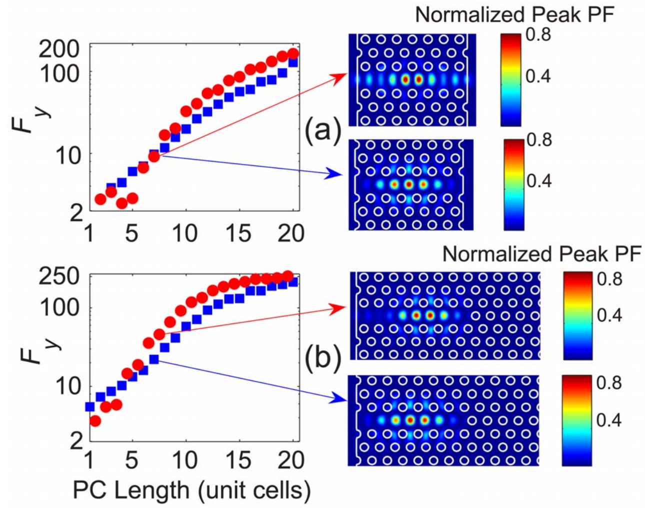

Fig. 3. (Color online) (a) Enhanced SE factor versus number of unit cells in a finite-size PC waveguide with air on either side. These are computed at the peak value over the frequency range shown in Fig. 2 and for the peak antinode position in the slab (see contour plots). The filled circles at the left are for the case when the truncation of the waveguide end is in between the nearest airholes on either side of the line-defect, and the filled squares at the left are the truncation of the waveguide end across the nearest airholes on either side of the line defect. The two insets show examples of the seven unit-cell guides for the peak Purcell factors, which are proportional to the $|E_y|^2$ field distribution, at the center of the slab in the xy plane for two different truncation ends in the seven unit-cell sized waveguide. (b) Similar to (a) but with a five-layer PC at one end.

the SE rates, which is a general effect for waveguides of longer than about eight unit cells. However, for shorter waveguides this scenario can actually be reversed [see emission factors in Fig. 3] but with less pronounced emission enhancements. With a completely flat interface termination, namely, a flat surface of air/semiconductor (without any partial airholes at the truncations ends), the enhanced emission factors are reduced from the values of their original structures. For example, for the same length of waveguide with a PC reflector, with 11.5 unit cells, we obtain $F_y=117$ for a flat interface as compared to $F_y=134$ in the corresponding original structure (with optimized truncation); for the waveguide length of 11 unit cells, the emission factors are $F_y=53$ and $F_y=71$, respectively, which is again somewhat less. We have also made a similar comparison for waveguides surrounded by an air medium on both ends and draw similar conclusions.

In terms of single-photon emission applications, one is also interested in the collection efficiency. To address this topic, we have calculated the total output-power coupling outside a waveguide facet from the QD emission as a function of the unit-cell number and for the two different truncation cases. In contrast to the clear monotonous behavior of enhanced SE with the unit-cell number, the power extraction efficiencies show a rather complex dependence in both types of waveguides as well as with different facet truncations. For example, for waveguides surrounded by an air medium on either end and with lengths ranging from 3 to 15 periods, the bidirectional output power that can be extracted from an embedded QD for the case *ii* facet exceeds 70% (these values are 3%–5% greater than in the waveguides with the case *i* facet), and for lengths ranging from 16 to 20 unit cells the output powers in both the cases remain around 65%–68%. For unidirectional waveguides, with either of the facet truncations, the power extraction efficiencies for waveguide lengths of 2–16 periods are in the range of 63%–70% and for longer waveguides these numbers reduce to 58%–60%. Altogether, these numbers seem very impressive since we have not yet optimized the device, and the Purcell factors are large enough for creating indistinguishable photons. Furthermore, interfacing with on-chip waveguide couplers are expected to be efficient as has been discussed elsewhere [10].

In summary, we have introduced a rigorous systematic numerical study of enhanced photon emission rates in finite-size planar PC waveguides. The single QD SE rate enhancements are strongly affected by waveguide length and facet truncation, allowing one to nanoengineer remarkably large Purcell factors with unprecedented precision.

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11. For this work, we have used "FDTD solutions," see www.lumerical.com.
12. L. Ramunno (University of Ottawa, Canada) and S. Hughes are preparing a manuscript entitled "Disorder-induced resonance shifts in photonic crystal nanocavities."