Hybrid Mie-Tamm photonic structure as a highly directional GHz single-photon source

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We present a photonic structure where Mie, Tamm and surface plasmon optical modes can be tailored to enhance the brightness of an embedded single-photon emitter. Contrarily to most proposals, the structure is designed for excitation and collection through the substrate side. The front surface can be used instead to arrange metal contacts which serve both, as electrical gates and optical mirrors. The design is particularized for InGaAs QDs on GaAs resulting in an outcoupled single-photon rate exceeding 3 GHz in a narrow cone of NA = 0.17. The fabrication tolerances are also discussed.

I. INTRODUCTION

A single-photon source with emission rate beyond 1 GHz is a key element in the field of quantum communications and linear quantum computation [1,2]. A major obstacle in obtaining efficient sources is not related with the quantum efficiency of the emission process but with the difficulty in extraction of the emitted photons from a planar surface. The high refractive index of semiconductors define a narrow solid-angle free of total internal reflection. Taking as example the GaAs-air interface, roughly 98% of the emitted photons are trapped within the sample. By placing a planar mirror in close proximity to the emitter, this limit can be raised increasing the extraction from 1/4πn² to 1/n², i.e. a factor four. [3] To further circumvent this limitation, three dimensional photonic structures are necessary, which either act on the near-field of the emission such as textured surfaces or micropillars, or in its far-field such as solid immersion lenses. [4] The extraction problem can be defined as a molding of the wavefront to funnel the light into a solid-angle as narrow as possible. If the extraction problem is combined with a high Purcell factor (F_p) [5], the brightness of the source can be increased even further. Micro-pillars and micro-lenses are very successful technologies to increase the brightness of single-photon sources. [6,7] The combination of a high fineness planar distributed-Bragg reflector together with a high aspect ratio of tapered micro-pillars allows for a very smooth extraction of the light from the semiconductor. The main drawback is the difficulty of fabrication and the complexity in addressing each micropillar individually for further post-processing. Micro-lenses also offer excellent collection efficiencies [8,9], but poor F_p mainly due to the large volume compared with the emission wavelength in the semiconductor. In addition, the reported size makes also difficult to build charge tunable devices and require transparent oxides if designed for upper extraction. A very good trade-off between collection efficiency and F_p is found in cylindrical distributed Bragg cavities also known as bull’s eye (BE). The best performance reported so far is for upper extraction with the BE written in a slab surrounded by air resting on a SiO₂/Ag support. [10-12]

In this work, we will analyze single-photon emitters embedded in asymmetric vertical optical cavities comprising a bottom distributed Bragg reflector (DBR) and a top metallic mirror. [13] The later can thus be used as an electrical contact to drive the emission or tune the single-photon emitter properties. Combined with an embedded excitation source underneath, a monolithic, stand alone and tuneable single-photon source can be realized. [14] Such planar asymmetric cavities harness optical Tamm states (OTS) and can exhibit very high Q values [15-18]. However, their planar geometry does not provide lateral confinement, a limitation which has been partially alleviated in the past by reducing the radial extension of the metallic layer. [19,21] Here, we propose to substitute the homogeneous cavity medium by a low refractive index dielectric layer embedding a high refractive index cylinder. This arrangement confines the light also in the plane and exhibits Mie-type resonances that can enhance the electric field [22]. The overlap of Mie resonances in the cylinder and the OTSs of the embedding dielectric layer offer new degrees of freedom which can be used to increase the F_p and to steer the emitted light into highly directional cones of light. Surface plasmon resonances near the metallic layer also play a role and shall be taken into account to avoid non-radiative losses. The sketch presented in Figure 1 graphically depicts the four main parts of the optical Mie-Tamm cavity (OMTC) just described. From top to bottom, we find the metallic layer, the dielectric layer, the cylinder that embeds the quantum emitter [23], and the λ/4 DBR. With these elements, the emission is steered backwards to the substrate where an optical fiber could be applied directly or using micro-optical elements, but its design is left out of the current study.

The design can be adapted for any material and wavelength combination. Without loss of generality, we will analyze the optimization of OMTC structures on GaAs embedding single InGaAs self-assembled quantum dots (QDs), SiO₂ dielectric layer and AlAs/GaAs DBR. These QDs show excellent purity [24] and indistinguishability [25]. Moreover, as these quantum emitters are based on III-V semiconductors, they can be integrated in photonic integrated circuits [26,27] and even in silicon substrates [28]. With these materials choice, we present in the following the optimum design parameters to extract from the sample 3.6 GHz single-photon rates in a narrow cone of NA = 0.17.

The paper is organized as follows. In section II, we describe the methods used to find the optimum parameters for our design. Section III presents the optimization results, the main properties of the OMTC structure and some design rules which results of the trade-off between fabrication complexity...
II. METHODS

The optical cavity is sketched in Fig. 1(a). The parameters are defined as follows. The top Au mirror thickness is set to 100 nm to reduce losses in the upper space and to reach the saturation region of the phase change [30]. The dielectric layer thickness is defined as $D = h + d$, where $h$ is the cylinder height and $d$ is an auxiliary parameter. The gap between the GaAs cylinder and the Au mirror is assumed to be occupied by a Au cylinder. Hence, GaAs and Au cylinders take the same radius ($r$) value. The QD is modelled as a dipole emitter perpendicularly oriented to the cylinder axis. It is located in its axis at a distance $z_{QD}$. OTSs tend to maximize the field at the mirror interfaces where also maximum enhancement of the emission might take place. However, a QD placed close to these interfaces might be either difficult to grow by self-assembly (DBR side) or suffer from spectral diffusion broadening and/or luminescence bleach (Au-GaAs side) [31, 32].

Two constraints are imposed, $z_{QD} > 10$ nm, minimum distance to the top DBR surface, and $z_{QD} < h + 50$ nm, minimum distance to the metallic cylinder. Both constraints are applied to maximize the fabrication feasibility of the device.

We exploit the axial symmetry of the system to speed up the solution of Maxwell’s equations, where the dipole emission asymmetry is handled by an expansion in Fourier modes [23]. The numerical solution is performed by the finite-element method with the commercially available software-package JCMsuite (ver 4.5) developed by the company JCMwave GmbH. The refractive indexes are extracted from Refs. [33] (GaAs and SiO$_2$), [34] (AlAs) and [35] (Au). Due to the many resonances that naturally occur in our system, the optimizations are performed in two stages using the monotonic basin hopping method with a 10% variation of the free parameters: $r$, $h$, $D$, $z_{QD}$. In the first stage, the structure is locally optimized from a starting point, taken as a seed. In the second step, the parameters are varied randomly within a prescribed range. Subsequent iterations finish when no improvement is found after a limited number of trials (five in our case). As local optimizer we use the BOBYQA algorithm [36] implemented in the NLopt library [37]. The whole optimization is performed with the library pygmo [38]. The objective function is defined to maximize the emission within a very narrow cone at the target wavelength of $\lambda_0 = 950$ nm. Without loss of generality, we set the cone aperture to $N_{AS}=0.17$, as a representative value of a highly directional emission. i.e. roughly a sixth of the critical angle ($N_{AC}=1$). As a figure-of-merit (FOM), we use the total photon number ($N_{ph}$) defined as the collection efficiency within a $N_{AS}$ times $F_p$. $N_{ph}$ has a straight-forward interpretation and if one assumes a typical exciton emission radiative lifetime of 1 ns in bulk GaAs ($F_p=1$), the optimized total photon numbers can be related to a extracted single-photon rate in the GHz range.

III. RESULTS

By inspection of Figure 1(a), we can envisage the two extreme cases of our design. For zero cylinder diameter, the structure is a SiO$_2$ OTC, and for very large diameters it operates as a GaAs-OTC. For cylinder sizes similar to the wavelength, Mie resonances are expected and we can think of an OMTC cavity. Resonances in a OTC follow the same pattern as in the Fabry-Perot (FP) cavity [16], i.e. $d_N = d_0 + N \lambda / 2n$, where $d_0$ is the minimum resonant thickness, $n$ is the refractive index and $N = 0, 1, \ldots$ is the FP order. As a seed value in the optimization, we have considered the thickness of the FP $N = 1$ in a SiO$_2$-OTC at 950 nm, i.e. $D = 460$ nm. Analogously, we set the initial height of the cylinder to the thickness of the same resonance in a GaAs-OTC, i.e. $h = 179$ nm. The other parameters are set to arbitrary initial values, $r = 200$ nm...
and \( z_{QD} = h/2 \) and let the algorithm find the optimal values. The optimal structure is found for \( r = 223.5 \) nm, \( h = 350 \) nm and \( D = 459 \) nm being the dipole located at 296 nm from the cylinder base. The optimal number of DBR pairs (\( N_{DBR}^{optimal} \)) is found to be 13 as explained below. Figure 1(b) shows the resonances found around 950 nm for \( F_n \) and \( N_{ph}^{optimal} \) for light collected within \( NAC \) and \( NAs \). At resonance, the maximum \( F_n \) is 13.6 and the maximum \( N_{ph} \) is 5.8 (3.6) for \( NAC \) (\( NAs \)), respectively. The lineshape of the spectrum also depends on the NA. At narrow collection angles, it exhibits a Lorentzian lineshape of 3.8 nm full-width at half maximum (FWHM), while, at the full extraction angle the line shape becomes asymmetric with FWHM=6 nm.

It is worth to compare the value \( N_{ph}^{optimal} = 3.6 \) found for \( NAs \) with that of two reference structures. In a substrate with a mirror, the collection efficiency is \( \approx 1/n^2 \). \[3\] For \( \lambda_0 = 950 \) nm, \( n_{GaAs} = 3.54 \), and assuming \( F_n \approx 1 \), we obtain \( N_{ph} = 0.080 \) for \( NAC \) and \( N_{ph} = 0.0023 \) for \( NAs \). The second structure is a GaAs-OTC of \( h = 179 \) nm, i.e. the asymmetric cavity described by Benisty et al. in Ref. \[13\] By placing the dipole at 10 nm from the DBR (lower bound considered in our calculations), a \( F_n \approx 1.4 \) results in the spectrum shown in Fig. 1(b) as a dashed line with a maximum \( N_{ph} = 0.061 \). Our design, introducing the Mie-Tamm hybrid structure, with the QD located at 50 nm apart of the nearest surface, improves the bare case by a factor 1500, and the perfected GaAs-OTC case by a factor 60. A clear signature of the advantages brought by the OMTC scheme.

A key element of the design is the DBR, as it is responsible for the OTS. Figures 1(c-e) show the evolution with increasing number of DBR pairs of the \( F_n \) and \( N_{ph} \) resonances found around 950 nm. The \( F_n \) peak intensity increases monotonically in the studied range, finding a maximum value of 21.1 for 20 DBR pairs [Fig. 1(d)]. Meanwhile, \( N_{ph} \) resonances have two different regimes where the peak intensity first increases up to 12-13 pairs depending on the NA and then decreases with the number of DBR pairs. This is the expected dependence for collection through the substrate side, since the transparency of the DBR mirror decreases with \( N_{DBR} \). In such case, there is a trade-off between the emission and collection enhancement throughout the substrate and the light storage in the cavity, which is also modulated by absorption at the Au gold mirror and other losses. Indeed, at the \( N_{ph} \) maximum, the total scattered power is 75 % (72 % in the downward direction) and the Au absorption is 25 % (\( NAC = NAs \)). Beyond that point, the absorption increases up to 42.5 %, as shown in Figure 1(f).

The resonance linewidth evolution is shown in Figure 1(g) as a quality factor \( Q = \lambda_0/\Delta \lambda \), where \( \Delta \lambda \) represents the FWHM. Again, the \( F_n \) linewidth shows a monotonic dependence, continuously narrowing in the studied range, while the \( N_{ph} \) linewidth first narrows down and then saturates beyond \( \approx 15 \) DBR pairs. This linewidth dependence determines how challenging will be the spectral matching between the QD emission peak and the cavity resonance. \[39\] Depending on the fabrication uncertainty, it could be beneficial to reduce \( N_{DBR} \) from 13 to 8 to increase the linewidth from 3.5 nm to 9.4 nm. The penalty being a reduction on \( N_{ph} \) from 3.3 to 1.2 GHz for \( NAs \). This trade-off between performance and fabrication yield can be anticipated from our analysis.

Further insight on the far-field distribution can be gained from the evolution of \( N_{ph} \) as a function of NA for varying \( N_{DBR} \), as depicted in Figure 2. The Figure follows the same color scheme as in Figs. 1(c-e). A bolder line is used for \( N_{DBR} = 13 \). The step rise of \( N_{ph} \) for small values of NA is a clear signature of the high directionality of the emission of our design, most of the light has been emitted for NA < 0.5. As shown in the inset by a contour polar plot, the far-field is concentrated in a very small NA area and lacks of azimuth dependence. The second step in \( N_{ph} \) comes from a very thin region around NA≈1.25. This, however, is emitted at an angle larger that the critical one and can only be extracted if an optical element is integrated in the back surface.

To understand how the optical mode structure varies with the geometrical parameters, we depict in Figure 3 the dependence of \( N_{ph} \) on either \( D \), \( h \) or \( r \), while keeping the other two parameters and \( z_{QD} \) fixed. The studied range is limited to 500 nm. The SiO\(_2\) slab thickness \( D \) shows two main resonances at 783 nm and 459 nm [Fig. 3(a)]. The free spectral range (FSR) is 324 nm, matching very well \( \lambda_0/2n \) in SiO\(_2\) [16,20]. The GaAs cylinder height \( h \) exhibits also two \( N_{ph} \) resonances in Figure 3(a), being the FSR=147 nm. This value differs by 13 nm from \( \lambda_0/2n \) in GaAs, as expected given the limited in-plane extension of the nanocylinder. Meanwhile, \( r \) shows also two resonances, being FSR=141 nm. The three dimensional nature of the nanocavity makes their study more involved. Indeed, we study the interplay between \( h \) and \( r \) in more details in Section IV.

This parameter exploration is done at fixed \( \lambda_0 \). To get a more comprehensive picture, the spectral dependence can be added to the analysis. Figs. 3(b,c) show contour plots of \( N_{ph} \) in logarithmic scale for different values of \( r \) and \( h \) and emission wavelengths.

The emission is negligible except at the design wavelength, \( \lambda_0 \), where the enhancement takes place at particular \( r \) and \( h \) values giving rise to the resonances di-
discussed above. Due to an exponential decay of $N_{\text{ph}}$ as soon as the cylinder size and wavelength depart from the optimal values, changing the cylinder radius alone does not provide an effective way to spectrally tune the OMTC and the QD in a broad range. Broad spectral tuning can still be done after growth, within the block band of the DBR ($\sim 100$ nm), reducing $h$ through etching to target smaller $r$ and $\lambda$. Alternatively, $N_{\text{DBR}}$ can be reduced as explained above to relax the spectral matching constraint.

The last parameters to be discussed are $z_{\text{QD}}$ and $x_{\text{QD}}$, the QD off-axis deviation. As shown in Figure 3(d) for the optimal geometry, $N_{\text{ph}}$ exhibits two maxima at $z_{\text{QD}}$ 134 and 295 nm. They are rather broad with FWHMs along the cylinder axis of 76 and 88 nm, respectively. They stem from the overlap with the field distributions shown in Fig. 4(a) which, as discussed in the next section, correspond to the cylinder Mie resonance of the OMTC structure. Similarly, $x_{\text{QD}}$ is peaked at the origin with a FWHM of 144 nm. The large value of FWHM is not surprising as in this type of Mie resonances the field tends to occupy a large portion of the nanocavity volume. The typical precision for in-plane positioning of quantum dots is around 40 nm [41,42,43], which could be used for deterministic coupling, although it is not necessary in our case.

The results just presented can be used to discuss the fabrication feasibility of the proposed design. Figure 3(e) shows the $N_{\text{ph}}$ evolution upon a change of the three most critical parameters around its optimum value. $h$ and $D$ are the most demanding with 3.1% tolerance each. This stems from resonance FWHMs of 11 nm and 14 nm, respectively. The less demanding parameter is $r$ exhibiting FWHM (tolerance) of 17 nm (7.6%). Reported experimental values of statistical variations of e-beam lithographic micropillars (30 nm on 2.0 µm diameter) and nanocylinders in metasurfaces (5 nm in 114 nm diameter) can be as low as 1.5% [44] and 4% [45], respectively. These values are below the required tolerance of $r$ in our case. Controlling the SiO$_2$ thickness within tolerance can be done by optically monitored dry etching to reach the target value from an overgrown sample. The results on Figure 3(e) indicate that even with deviations twice as large, $N_{\text{ph}}$ can reach 0.8 within NA$_S$ (or 800 MHz single-photon count rates extracted from the sample).

Depending on the aspect ratio of the structure, the surface roughness has a great impact on the optical properties. In the case of nanopillars with large aspect ratios, diffraction at the wall roughness produces scattering of the guided mode into other modes resulting in a reduction of the Q-factor [6]. As the height of the micro-pillar decreases and the diameter increases towards a shallow cylinder, the FSR between adjacent Mie resonances becomes larger and hence a weaker scattering by the surface roughness is expected. Similarly, the exciton linewidth can be affected by surface states and traps at a rough surface. Liu et al. [45] performed a study of these issues on QD based photonic nanostructures including surface passivation with Al$_2$O$_3$. They showed that the quantum efficiency is not affected at all in the proximity of dry-etched surfaces 50 to 300 nm away from the QD. At 150 nm the peak broadens by a factor 1.38 and at 300 nm, the surface does not affect the linewidth anymore. In the whole range, the $g(2)(0)$ value remains constant. In our case, we find the optimal $r=223.5$ nm, and thus a broadening factor of the order of 1.2 in the exciton emission line could be expected. From this discussion, we believe that OMTC designs like the one presented here are feasible from the physical and fabrication point of view.

IV. DISCUSSION

The interplay between the OTS and the Mie resonances can be inferred from the field distribution shown for the optimized structure in Figure 4(a). The white lines indicate the different regions depicted in Fig. 1(a). In the SiO$_2$ slab (top-right) a node line spans parallel to the substrate. This corresponds to the OTS resonance used as seed in the optimization, i.e. a full oscillation of $\lambda_0/2$ in SiO$_2$ fits within the structure. In the DBR region (bottom half region) an oscillation of the electric field in phase with the DBR period is found. Indeed, despite the three dimensional character of the cylinder, the wavefront is parallel to the DBR’s interfaces leading to the narrow directionality of the emission. The field distribution inside of the cylinder clearly shows the excitation of a Mie resonance as anticipated in the discussion of $x_{\text{QD}}$. In this particular case, $|E|$ shows two ring structures and $|H|$ shows two anti-nodes. This field distribution is characteristic of a magnetic multi-
pole resonance \[47–49\] and has been previously reported for a horizontal dipole located near the top or bottom surfaces in free-standing cylinders \[50\].

The properties of the OMTC cavity are better understood from the evolution of \(F_p\) as a function of \(r\) and \(h\) for fixed \(d\), i.e. \(D\) changes with \(h\). Figure 4(b) shows the corresponding contour plot with all the resonances excited in the system. The white arrow points to the optimal one. We recall that \(r\) determines whether the structure behaves as a SiO\(_2\)-OTC (\(r \ll \lambda_p\)) or as a GaAs-OTC (\(r \gg \lambda_p\)). For \(r = 50\) nm discrete resonances appear with a FSR of \(\lambda_p/2\) corresponding to the SiO\(_2\)-OTC and indicated by vertical white dashed lines. At \(r = 450\) nm, another family of resonances appears, with an FSR of \(\lambda_p/2\), which is associated to the GaAs-OTC by a series of vertical white dotted lines. The modal structure of the cylinder offers enough flexibility to smoothly connect both limits. The optimal structure appears when \(h\) gets close to the GaAs-OTC FP \(N = 2\). Around this \(h\), the SiO\(_2\)-OTC FP \(N = 1\) mode is also excited. This explains why \(|E|\) exhibits two nodes in the cylinder while only one in the SiO\(_2\) slab in Fig. 4(a). The Purcell factor contour plot also reveals a series of horizontal resonances crossing the Mie resonances at regular \(r\) intervals. They are related with the excitation of surface plasmon polaritons at the GaAs/Au interface as explained below.

Figure 5(a) shows a line plot of \(F_p\) as a function of \(r\) fixing \(h\) at the optimal value. The blue line stems for the absorption in the Au mirror calculated as the fraction of the total emitted power as explained above. We distinguish two series of mode peaks labelled \(O_{1n}\) and \(M_{mn}\), respectively. Their different nature is revealed by plotting in Figs. 5(b-g) the cross-sections of \(\Re(E_y)\) in the XY plane (top) and XZ plane (bottom) for each mode. The field distributions in (b), (d), (f) and (g) are clearly confined in the GaAs/Au interface, while those in (c) and (e) occupy the volume of the GaAs cylinder. In view of these results, the latter are attributed to Mie resonances of different magnetic multipole order (\(M_1\) and \(M_2\)) while the former can be related to surface plasmon polaritons (SPPs).

Our analysis reveals that, in the region of the GaAs/Au interface, the metallic contact acts as a circular plasmonic patch nanoantenna \[51\]. In our configuration, the dipole is ori-
Hence, we can assume that the dependence is very weak.

$$2\Re(k_{SPP})r_n + \phi' = 2\pi n,$$

where $r_n$ is the $n$-th radius at resonance, $\phi'$ is the phase origin, $k_{SPP}$ is the SPP wavevector, and $x_n$ is the $n$-th zero of the $J_1$ Bessel function. The phase $\phi'$ depends on $r$, but, as a first approximation, we can assume that the dependence is very weak. Hence, $r_{n+1} - r_n = (x_{n+1} - x_n)/\pi k_{SPP}/2$. In addition, verifies that $(x_{n+1} - x_n) \approx \pi$ for small $n$, and therefore the FSR is very close to $\lambda_{SPP}/2$, as expected. This is final confirmation of the nature and position of the different SPP resonances found in our system.

One needs to be aware of the presence of these SPP resonances when designing an OMTC structure. They can introduce large parasitic losses jeopardizing the enhancement of $F_p$ and $N_{ph}$ produced by the combination of Mie and OTS resonances. So, even if our design is fully scalable to other wavelengths, e.g. 1.3 µm or 1.5 µm just by rescaling the DBR, $r$, $h$ and $D$ accordingly, some care needs to be taken in case of the material dispersion introduces the unwanted overlap between SPPs and Mie-resonances just described. Otherwise, a penalty in performance would be paid.

We finish this Section reviewing the main assets of our approach. The backwards collection through the substrate side allows to use a metallic optical mirror and ohmic contact to drive and tune electrically the emission. The design relies on a semitransparent DBR located underneath the QD, which enables optical excitation through a built-in or external laser diode. Secondary micro-optical elements can be located in the substrate to excite and/or collect the photoluminescence, which would not interfere spatially with the primary photonic nanocavity embedding the QD. Compared with photonic crystal microcavities, the removal of material surrounding the cylinder reduces the chances of unwanted luminescence from nearby QDs contributing to the optical mode. Also, the Mie resonance in-plane extension fills a great ratio of the cavity cross-section increasing the chances of good spatial overlap in low density QD samples without requiring deterministic methods. From the performance point of view, the directionality of the emission is superb and allows large extraction single-photon rates within low NA even with moderate Purcell factor values. In addition, the design is fully scalable and manufacturable with current micropattern fabrication techniques.

V. CONCLUSIONS

We introduce and analyse a photonic structure to enhance the brightness of single-photon sources with very high efficiency. Via a global optimization method, we find the optimal structure parameters for the case of InGaAs QDs embedded in GaAs. From the analysis of the resulting structure we show that the enhancement is based on the cooperation of Tamm and Mie resonances intertwined in our design. We predict a $N_{ph}$ of 3.6 for a narrow extraction cone of NA≈ 0.17 and 5.8 for the critical angle extraction cone (NA≈ 1) which boosts the extracted single-photon rate at the GHz range. These values are significantly larger than those attainable in a bare optical Tamm cavity or a bare Mie structure of comparable size. Therefore we term our proposal as an Optical Mie-Tamm Cavity (OMTC).

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