A new III–V nanowire-quantum dot single photon source with improved Purcell factor for quantum communication

Shahram Mohammadnejad1 · Amine Mahmoudi1 · Hossein Arab1

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Abstract
In this work, the finite difference time domain method has been utilized to simulate the propagation emission from PbS quantum dots in a hexagonal InP nanowire as a single photon source. The effect of height and radius of the nanowire as well as the location and orientation of the dipole source in the Purcell factor and Quality factor of the nanowire have been investigated. A broadband electric dipole source has been used to model the quantum dot and the effect of shape and radius of PbS quantum dot have been investigated in the final results. The conclusive structure has been optimized to a nanowire with hexagonal cross section with radius of 220 nm and height of 10 μm. The emission peak obtained above 1 μm with Purcell factor of 5.45 which is in good agreement with cases have been used as single photon source in quantum communications.

Keywords Quantum dot · Nanowire · Single photon source · Purcell factor · Quality factor · Telecommunication

1 Introduction
Recently, high-speed and reliable data transferring and processing have attracted researchers’ attention in the field of quantum information technology. In recent studies, one of the typical candidates for single and entangled photon sources, are semiconductor quantum dots (QDs) (Nozaka and Mukai 2016). In this way, self-assembled semiconductor QDs created by Stranski-Kranstanov (SK) (Anderson et al. 2021; Baskaran and Smereka 2012; Xiang et al. 2017) method, have good potential to be applied in practical systems of light sources. However, their solid state environment brings up some challenges (Artioli et al. 2019).

In order to produce entangled photon pairs, QDs with high structural symmetry are needed that is one of the fundamental technologies in quantum processing. While self-assembled QDs have been utilized widely, but their symmetry is significantly low, not only in the direction perpendicular to the substrate, although in the horizontal direction due to the adatom diffusion length variations in substrate direction. Hence, many studies have
been done in order to find some methods to improve structural symmetry. Temperature control (Bietti et al. 2020), the use of magnetic fields (Stevenson et al. 2006) and growth with strain-reducing layers (Mukai and Nakashima 2008; Mukai et al. 2009) are some of the mentioned methods in the literature (Nozaka and Mukai 2016).

Recently, nanowires (NWs) have received researchers’ attention due to their special optical and electronic characteristics. They have been of great interest in nano-sized electronic and optoelectronic devices because of strong two dimensional confinement that they cause in electrons, holes and photons (Wang et al. 2006). Additionally, for efficient production of single photons, quantum emitter has been coupled to a resonance mode of a cavity or NW waveguide with high Quality factor (Lounis and Orrit 2005). Single photon emission from QDs coupled to NWs has been widely studied for wavelengths lower than 1 μm (Cirlin et al. 2018; Holmes et al. 2014; Leandro et al. 2018; Yu et al. 2014). Furthermore, during recent years some cases of NW-QD structures with the emission wavelengths above 1 μm has been reported to be applied in telecommunications (Dorenbos et al. 2010; Reimer et al. 2012). These types of structures are suitable candidates for the light sources because of their doping, shape and material controllability (Dorenbos et al. 2010).

In another side, QDs can be produced in a flask by chemical methods. These types of QDs which have been called colloidal QDs (CQDs), have high three-dimensional symmetry (Nozaka and Mukai 2016). Also, because CQDs like PbS and PbSe cover a wide range of wavelengths (Fushman et al. 2005), these QDs can be used in optical telecommunication wavelengths. Moreover, their production cost also is low (Nozaka and Mukai 2016). For this reason, CQDs are attractive for the optoelectronics and also the quantum information technology.

QD position control is crucial to achieve an ideal QD-NW coupled system. The position of the SK QDs is controlled using a processed substrate, but this method seems undesirable, because the preprocessing destroys the quantum efficiency by producing crystal defects. While to control the position of CQDs, a nano-hole is made using screening probe microscopy (SPM) on the Si substrate to trap a PbS CQD. SPM position control technology has the maximum accuracy of single atom (Stroscio and Eigler 1991; Fölsch et al. 2014), and of course this method can be used to integrate the devices with Si photonic technology (Nozaka and Mukai 2016).

Despite recent developments, another serious limitations of IR sources based on QDs for use in telecommunications, is their low modulation speed. Regardless of the electrical constraints, the main limitation of the modulation speed is the low spontaneous emission rate of the PbS QDs, which have a typical lifetime of about a few microseconds. This low radiative recombination rate has been attributed to the unconventional highly degenerated band structure of QDs or to the large dielectric screening of excitons in lead-based salts; The mechanism, however, is not entirely clear.

To solve the problem of low lifetime of Lead-based QDs, they have been integrated with waveguides, specially the optical cavities with low mode volume to improve the radiative characteristics of emitters by Purcell effect. Purcell effect is to increase the radiative and non-radiative transition rates of quantum emitters by increasing the local density of optical states in the location of emitter (Akselrod et al. 2016).

First demonstration of coupling CQDs to photonic crystal cavities has been showed by Fushman et al. in 2005. They used PMMA-soluble PbS QDs deposited on cavities with AlGaAs membrane as a wide-band on-chip source to characterize cavities (Fushman et al. 2005). In another investigation has been done by Akselrod et al. in 2016 in the field of IR light emitting diodes, they decreased the emission lifetime of QDs from microsecond to nanosecond by coupling PbS QDs to colloidal plasmonic nanoantennas.
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based on metal nanocubes, which has been done by increasing radiative decay rate and finally, it led to an increase in the quantum efficiency of the nanoantenna (Akselrod et al. 2016). There has also been a lot of research in recent years on PbS/CdS core/shell QDs (Elsinger et al. 2019; Huang et al. 2017).

Many studies (Deshpande et al. 2013; Wang et al. 2001; Deshpande and Bhattacharya 2013) have been performed on the effect of the in-plane point dipole position whose polarization is perpendicular to the axis of the NW. This situation is observed experimentally in high-efficiency single photon sources (SPSs) based on a self-assembled QD in a photonic wire (Friedler et al. 2009). Assuming that the lateral confinement is not important (as in the behavior of an axial quantum well), a QD can be modeled with an in-plane dipole source in a wurtzite material (Henneghien et al. 2009).

Although FDTD is a classic calculator, it can be a tool for optimizing optical devices and components of quantum photon experiments. One of the major design challenges in this field is the optimization of light collection from solid state QDs, which are called SPSs and are usually achieved through nanopillar cavities.

It is not possible to model a single photon in a classical way, however an ideal SPS produces completely uncorrelated photons, so it can be modeled using an incoherent non-polar source and how many photons on average Collected by fiber can be measured.

In this paper, we attempted to simulate a PbS QD inside a hexagonal InP NW to obtain the optimum Purcell factor, Quality factor, and electric field intensity of the emitted mode with respect to the emitted wavelength per radius and height of the NW, shape and size of the QD as well as the location of QD along the NW axis. In this work, the NW material had to be selected in such a way that the band gap of the NW was larger than the band gap of the QD material to achieve the quantum confinement of the QD. To do this, we used InP NWs whose lattice constant is close to that of the PbS (Fig. 1).

![Fig. 1 band gap diagram versus lattice constant for some semiconductor materials (Downs and Vandervelde 2013). We added properties for PbS QDs with diameter of 15 nm (red circle)](image-url)
2 NW modeling

A NW is inherently a Fabry–Perot cavity with two surfaces that act as reflectors. Semiconductor NWs Due to their crystalline structure, have a non-circular cross section, which makes it very difficult to solve Maxwell equations for waveguide modes inside the NW. For this reason, by approximating the hexagonal cross section instead of the circle, it can be able to obtain low-order waveguide modes with good accuracy. In 2005, Nobis and Grundmann (Nobis and Grundmann 2005) by considering similar refractive indices for both circular and hexagonal NW structures, expressed the scaling relationship of their cross-sectional surfaces as follows:

\[
\frac{3\sqrt{3}}{2} L^2 = \pi a^2
\]

In this relation, “a” is the radius of the circular NW and L is the radius of the hexagonal NW, which is: 1.1a = L.

The refractive indices of the nanowire and the surrounding medium are \(n_1\) and \(n_2\).

Within the non-absorption spectrum, the waveguide properties of NWs can be retrieved by solving Maxwell equations as follows:

\[
\begin{align*}
(\nabla^2 + n^2 k^2 - \beta^2) \vec{c} &= 0 \\
(\nabla^2 + n^2 k^2 - \beta^2) \vec{n} &= 0
\end{align*}
\]

where \(k = 2\pi/\lambda\); \(\lambda\) is the wavelength of light in vacuum and \(\beta\) is the propagation constant. These equations can be solved with the following eigenvalue equations in cylindrical coordinates for the modes \(HE_{vm}\) and \(EH_{vm}\) as follows:

\[
\begin{pmatrix}
J_v'(U) + K_v'(W) \\
UJ_v(U) + WK_v(U)
\end{pmatrix}
\begin{pmatrix}
J_v'(U) + n_2^2 K_v'(W) \\
UJ_v(U) + n_2^2 W K_v(U)
\end{pmatrix} = \left(\frac{\nu \beta}{kn_1}\right)^2 \left(\frac{V}{UW}\right)^4
\]

In this equation, \(J_v\) and \(K_v\) are Bessel functions. \(U = a(k_0^2 n_1^2 - \beta^2)^{1/2}\), \(W = a(k_0^2 n_2^2 - \beta^2)^{1/2}\), and \(V = ak_0(n_1^2 - n_2^2)^{1/2}\) are waveguide parameters and \(k_0\) is known as the wavenumber in free space and we have \(k_0^2 = \omega^2 \mu_0 \varepsilon_0\), where \(\mu_0\) and \(\varepsilon_0\) are the permeability and permittivity in vacuum, respectively (Ma et al. 2013).

By solving these equations numerically, NW waveguide modes can be obtained. When the diameter of the NW is less than the wavelength of the guided light, new properties are created in the NW that lead to severe light limitation inside it and the light can be easily conducted in it. It also exhibits a single-mode performance for a specified value of NW diameter, and usually occurs when the NW diameter is less than \(\lambda/n_1\) (Huang et al. 2017). However, if the NW is too thin, it will show poor reflection and will have a lot of leakage losses.

3 Simulation results

In this paper, we have used NWs with hexagonal cross-section and substrates of the same material as InP. Although circular and hexagonal NWs are almost identical, hexagonal NWs eliminate degeneracy of \(HE_{11}\) mode due to reduced structural symmetry. Also
relatively low reflection from the end face, limits the Q-factor (which is the stored energy divided by the energy dissipation per cycle) of F−P cavity semiconductor NW to below a few hundred.

In addition, although semiconductor NWs have very low surface roughness, they usually have very high waveguide losses (e.g. SnO₂ nanoribbon, 10–80 dB/cm in the 500 nm wavelength range (Law et al. 2004)) compared to glass nanofibers (e.g. SiO₂ nanofiber, 1 dB/cm in the 600 nm wavelength range (Tong et al. 2003)). In our work, we set the wavelength of the dipole source to be broadband from 830 to 1420 nm. The losses for the $HE_{11}$ mode for the finely structured NW are 0.13 dB/cm. We obtained more losses for other guiding modes compared to $HE_{11}$ mode. Given that for nanophotonic applications, the effective length required for semiconductor NWs is usually a few ten micrometers, losses at this level are acceptable.

Due to the difference in the arrangement of the atoms in the two types of crystal structures of zinc-blend and wurtzite, zinc-blend NWs emit light with polarization along the NW axis, while in wurtzite NWs, the emitted light has polarization perpendicular to the growth axis of the NW. In the simulations, we have modeled the single-photon emission from the QD with an electric dipole located on the NW axis, which allows dipole orientation as shown in Fig. 2. In fact, the radiative properties of a quantum emitter can be considered using the classical electromagnetic effect, assuming that the quantum emitter operates as a point dipole with time-varying dipole moment. The dipole source in FDTD can be used to study these radiative properties in a homogeneous or a non-uniform environment where emission is affected by scattering and absorption of light by near dipole structures.

The angular distribution of the power emitted by a dipole placed in vacuum, is a function of $\sin^2 \phi$, which for the $\phi = 0$, orientation, is in the dipole’s orientation. Therefore, it is expected that light is emitted perpendicular to the NW axis and no light is observed in the direction parallel to the dipole, however, due to the dielectric environment around the dipole, the emission profile is modified.

The intensity of the electric field is also a function of the light transverse k-vector, which is perpendicular to the direction of photon emission (Fig. 3). Also, the emission angle $\phi$ as $k = \arcsin \phi$ is related to the k-vector. The minimum and maximum electric field intensities per $k=0$ are obtained when the dipole is oriented parallel to the NW axis and perpendicular to the NW axis. We examined Purcell factor and Quality factor by changing

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**Fig. 2**  a Illustrations of various types of dipole source orientation within the NW structure. b Theta and phi angles
the dipole source polarization angles in FDTD. When an electric dipole is located inside a nanowire, the Purcell factor and the Quality factor are changed, depending on the orientation of the electric dipole in the x, y, and z axes. As shown in Fig. 4a, the values of the Purcell factor and the Quality factor are maximum in the direction which the dipole polarization is perpendicular to the nanowire axis and along the x-axis. As shown in ref Lukosz and Kunz (1977), angular distribution of emitted radiation from an electrical dipole embedded within a nanocavity has a $\sin^2 \theta$ dependence in vacuum environment in which $\theta$ represents the angle between nanowire axis and dipole’s emitted photon direction and when $\theta = 0$, the emitted photon extracts from the nanocavity exactly on the nanowire axis direction. On the other hand, it has been showed that the generated photons from the dipole will be emitted perpendicular to the dipole direction and there will be no emitted photons parallel to the dipole direction (Bulgarini et al. 2014). However, a dielectric environment or an interface around the dipole, can slightly improve the emission profile (Bulgarini et al. 2012). Hence, for achieving the maximum emission power from an electrical dipole, the direction of the dipole must be adjusted perpendicular to the nanowire axis in order to emit its photons with maximum power. This process has been confirmed in Fig. 4a as well and it can be noticed that the maximum Purcell factor and Quality factor values of the electrical dipole are obtained when it is oriented along the x-axis and perpendicular to the nanowire axis (z-axis). Besides, this effect can be understood by simulating the electric field profile of emitted photons and solving the Maxwell’s equations for the electrical dipole oriented parallel and perpendicular to the nanocavity axis, too (Bulgarini et al. 2014). In Fig. 4c, it can be seen in which wavelength the peaks of Purcell factor and Quality factor occur. We also obtained the highest electric field intensity for the same condition shown in Fig. 4b. In Fig. 4b, considering the nanowire dimensions of $h = 10 \, \mu m$ and $r = 220 \, nm$, a dipole source is placed in the center of the nanowire with the angles of theta 90 and phi 0, the frequency of which is set at 830 nm to 1423 nm. To obtain the electric field with the mentioned conditions, a PML layer was placed around the structure with a distance of at least half a wavelength to model the absorber boundary conditions around the nanowire. In this modeling, the distance between the PML layers should be sufficient to minimize the reflections at the boundaries. The electric field of the structure was obtained using a frequency domain field
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and power monitor shown in Fig. 4b. The maximum electric field intensity occurs at the center of the structure due to the emission mode $HE_{11}$, which is equal to 16 a.u. (arbitrary unit).

Figure 5 shows the Quality factor and the Purcell factor based on the changes in the radius of the NW for a dipole source located at the center of the NW with a height of 10 μm and orientation perpendicular to its axis. Peak wavelengths are always above 1000 nm for all radii. As can be seen from the Fig. 5, at low radii, for a radius of 160 nm, a peak is observed in Purcell factor and Quality factor. The peak wavelength obtained for a radius of 160 nm is equal to 1047 nm; however, the intensity of the electric field observed at this peak is weak. As the NW radius increases from about 180 nm, both factors increase.

In dielectric environments, the spontaneous emission rate can be changed (Scully and Zubairy 1999; Loudon 2000). The spontaneous emission rate depends on a parameter called optical local density of states (LDOS) (Wei et al. 2015) and this is shown in Fermi’s Golden Rule (Novotny and Hecht 2012). In homogeneous medium-sized environments, the spontaneous emission rate is a constant, depending on the polarity of the light source and the permittivity of the medium, but when the dimensions of the structure approach to the levels close to the emission wavelength, the LDOS value changes and is spatially controlled. As a result, the spontaneous emission rate of the device can be controlled based on the geometry of the device.

Fig. 4  
(a) Quality factor and Purcell factor versus variation of polarization angle of dipole source.  
(b) The intensity of electric field per theta=90 and phi=0.  
(c) Purcell factor and Quality factor versus wavelength for three dipole orientations
In InP nanowire, which act as microcavity to emit light produced in quantum dot, increasing the nanowire radius leads to a significant increase in LDOS, thereby improving the spontaneous emission rate. This leads to an increase in the Purcell factor and the Quality factor as shown in Fig. 5 (Zhang et al. 2020). This results in a better coupling of the radiation produced by quantum dot to the fundamental mode of the waveguide, and by better limiting the generated excitons, the efficiency of the device is significantly increased. The point that can be seen in this figure is the decrease in the values of Purcell factor and Quality factor in the dimensions of less than 180 nm, which is interpreted as a result of the cavity effect. When the nanowire radius is less than 180 nm, the microcavity will not be able to support the fundamental mode of $HE_{11}$. This condition causes the electric field intensity to be weak in radii less than this value and as a result the mode volume of the device is very small and due to the inverse relationship between the Purcell factor and the mode volume, this issue reduces the Purcell factor and the Quality factor (Tang et al. 2016). By increasing the radius of the nanowire to more than 180 nm, the fundamental mode of $HE_{11}$ appears in the nanowire, and as a result, the intensity of the electric field and the Purcell factor of the device increase. This will continue with further increase of the nanowire radius and higher modes such as $TE_{01}$ and $TM_{01}$ will be formed in the nanowire.

The Purcell factor in a single photon emitter can be determine as follow (Purcell et al. 1946):

$$F_p = \frac{3}{4\pi^2} \left( \frac{\lambda}{n} \right) \left( \frac{Q}{V} \right)$$

In this equation, $\lambda$ is the wavelength of emitted light in the environment, $n$ is the refractive index of the environment, $Q$ is the Quality factor and $V$ is the volume of the mode, which is calculated by the following relation:

$$V = \int \frac{\epsilon(r)E^2(r)dr}{\epsilon_ME^2_M}$$

In this equation: $\epsilon(r)$: the relative dielectric constant at the position $r$. $E(r)$: the electric field of the light at the position $r$. $\epsilon_M$ and $E_M$: corresponding values at the position of the maximum light intensity.

In the following, we examine the effect of NW height on Quality and Purcell factors. In these simulations, we examined the results with a NW height sweep from 3 to 13 μm (Fig. 6). Maximum Purcell factor which observed, is strongly dependent on the NW height. In this structure, as the height of the NW increases, the peaks of the structure shift to higher wavelengths. So that for NW heights lower than 8 μm, the wavelength of the maximum Purcell factor is less than 1000 nm. With increasing NW height from 8 μm onwards, two peaks can be seen in Fig. 6, obtained for 10 μm and 11 μm heights, respectively, and their Purcell factor and Quality factor values differ very little.

According to the diagrams in Figs. 5 and 6, the values of radius and height of NW was selected as 220 nm and 10 μm, respectively and then, we obtained the profile of electric field intensity as shown previous in Fig. 4.b. The selected guiding mode in the NW was $HE_{11}$ mode which has been shown in Fig. 7. This figure is just to show the
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Fig. 6  a Purcell factor and Quality factor versus variation of the NW height (the NW radius is considered to be 220 nm). The variation of Purcell factor and Quality factor versus wavelength have been shown in Figures (b) and (c) respectively.
emission mode $HE_{11}$. Considering that in all the results of the simulations, the desired mode is $HE_{11}$, so that there are the least losses in the structure.

To observe the effect of dipole source position on Purcell factor and Quality factor, we swept the dipole source from $z = -4.5$ to $z = 4.5$ µm. The two diagrams obtained from this sweep (Fig. 8a) change almost symmetrically and three peaks can be seen in it. As shown in Fig. 8a, when the source is more than 2.5 µm away from the center of the NW, the Quality factor decreases. However, the Purcell factor did not decrease sharply and did not fluctuate more except at the origin of the NW. The maximum value of Purcell factor is obtained when the dipole source is located in the center of the NW ($F_p \approx 5.45$). Since the excitation efficiency of NW modes depends on the intensity of the field of a mode at the location of the dipole source, by placing the source in the center of the NW axis, the electric field also intensifies. As shown in Fig. 8, the maximum values of the Purcell factor and the quality factor occur when the quantum dot is located exactly at the center of the nanowire, in other words, the structure is designed symmetrically. When the symmetry of the structure is lost, the electron states will not change noticeably on either side of Quantum Dot, but the hole states are strongly affected by this structural asymmetry. In symmetric structures, the output emission spectrum is more intense than the emission spectrum in asymmetric structures, which indicates a higher efficiency in symmetric structures and indicates a higher Purcell factor and quality factor in symmetric structures. Purcell and Quality factors in asymmetric structures do not arise from anisotropic exchange interactions between the two regions, but the hybridization of the hole states appear in these asymmetric structures and reduce the device efficiency. In reference (Bouwes Bavinck et al. 2016), the effect of symmetric position of quantum dot within the nanowire has been studied and it has been claimed that the symmetric structures represent only one strong single z-polarized excitonic peak which predominantly originated from the second and third excited hole states ($h_2$ and $h_3$) while the ground hole state ($h_0$) and first excited hole state ($h_1$) showed
weak emissions and remained dark. By ruining up the symmetry, two weaker splitted z-polarized peaks were appeared which originated from hybridized character of the hole states and this time, the first excited hole state \( (h_1) \) participated in an optically transition with a s-shell electron while the ground hole state \( (h_0) \) still remained dark. By comparison of the emission spectrums in symmetric and asymmetric devices, it could be noticed that symmetric structures have greater emission peaks because of higher order excited hole states participation in emission spectrum and this fact have been emphasized by the investigation of Purcell and Quality factors in symmetric and asymmetric devices which are shown in Fig. 8 (Bouwes Bavinck et al. 2016; Arab et al. 2020; Bayer et al. 2002).

Although in FDTD simulations the QD is modeled with a dipole source, we nevertheless placed a QD of PbS material in three types of shape (Fig. 9) (so that the dipole source is in the center of the QD) and selected a finer mesh for its structure and so we tried to include the effects of the QD material in the simulations. The simulation results show that for circle QDs with a radius of \( \sim 8 \text{nm} \) we will obtain the highest value for Purcell and Quality factors (Fig. 10); Although PbS QDs built in practice, are spheres. According to the simulation, by increasing the radius of the sphere QD, the Purcell factor decreases with a gentle slope.

The characteristics of the final structure are summarized in Table 1. The shape of the final structure is also shown in Fig. 11.

In linear systems, the resonator response to external excitation does not depend on the excitation source. In the frequency domain, the system response is related to the source as follows:

\[
t(\omega) = h(\omega) \cdot i(\omega)
\]

where \( t \) is the response, \( i \) is the source signal and \( h \) is the transfer function that relates both quantities for each angular frequency \( \omega \). The quantity \( h \) is an intrinsic property of the resonator and is the impulse response of the system, ie the response when \( i(\omega) = 1 \), or \( i(t) \) is a delta function.

The ideal method for calculating \( Q \) is to calculate \( h(\omega) \) and extract \( Q \). This is what we do when the cavity is a low-Q cavity. We then calculate \( h(\omega) \) by

\[
h(\omega) = t(\omega) / i(\omega)
\]

A cavity is called a low Q cavity when the electromagnetic fields decay completely during the simulation time in FDTD. In this case, the Quality factor can be determined from the Fourier transform of the field by finding the resonance frequencies of the signal and measuring the full width half maximum (FWHM) of the resonant peaks. We can then use \( Q = f_R / \Delta f \) where \( f_R \) is the resonant frequency and \( \Delta f \) is the FWHM.

Despite the fact that photoluminescence is a quantum mechanical effect, we can consider the radiative properties of a quantum emitter as classical electromagnetism radiation, assuming that it acts like a point dipole with a time-varying dipole moment. Hence, in FDTD simulations, an electrical dipole source can be utilized to study these emission characteristics in homogeneous or non-homogeneous environments. In other words, the actual behavior of this process is based on quantum mechanics, practically, in which the emitted photons are considered classically in the electric or magnetic point dipole source.
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(a) Purcell & Quality Factor Vs Dipole Source Position

(b) Wavelength (nm)

(c) Quality Factor
simulations. This dipole source is located in the quantum dot position and models the emitter radiation properties. For investigation of emission spectrum for this device, the wavelength of simulations was set to 830–1423 nm and the power intensity of simulation was chosen to 1 amplitude which is equal to 1 Femto Watt in 3D simulations.

The simulations performed at room temperature (300 °K) in vacuum conditions without applying any external fields. Additionally, it should be noticed that in the FDTD simulations, temperature variation will affect the results if temperature-dependent index-perturbation materials are used. As a result, the values of index-perturbation materials in these simulations will only affect the material explorer values and have no effect on the emission spectrum or other reported results. We used a Q-analysis monitor consisting of several time monitors to observe the emission spectrum of the structure. We set this analysis object to consist of 15 point monitors to reduce the chances that a monitor is placed at a node in the mode profile of a cavity mode yielding a weak signal. Also, the initial transients of the source are neglected by setting the “start time” for the time monitors to 200 fs. The “start time” for the time monitors is the time at which the monitors begin recording data. Our simulated cavity was considered a low Q cavity because the electromagnetic fields fully decay over simulation time.

Also, given that the dipole source is located in a dispersive medium, the emitted power from the source is calculated by measuring the power flow out of a small box of frequency domain field and power monitors surrounding the source, which gives the Purcell factor. The transmission box analysis object from the Object library can be used for this purpose which have a very close match with the Purcell factor spectrum obtained from the calculations of the dipole source.

Numerical simulation results are always associated with some errors, and the reduction of these errors is often involves increased simulation time and memory. We tried to reduce these errors by performing convergence tests, including the number of PML layers, the distance of the layers from the structure, the simulation time and the structure meshing.

In these convergence tests, increasing the number of PML layers reduced the reflections from the PML. Also, determining the appropriate mesh for the structure was chosen according to the system used for running the simulation. In these types of simulations the mesh order of the internal structure must be less than the outer structure in order to simulate it correctly. Due to this reason, the meshing in the quantum dot range was finer than the meshing in other parts of the structure. In addition to these convergence tests, we tried to fit and adjust the imported sample data model over the frequency range specified by the source to create a lossless material.

The Purcell spectrum of the final structure for the circle QD (Fig. 12a) shows that the highest amount of Purcell factor occurs at 1024.8 nm, with a Quality factor of 295.25 at
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this wavelength (Fig. 12b). The intensity of the electric field at this wavelength is propagated in $HE_{11}$ mode which has been shown in Fig. 12c. This figure shows the electric field...
of the final simulated structure considering the QD in the form of a circle with a radius of 8 nm. The electric field intensity in this emission mode is maximum at the center of the structure and has a value of 15a.u. Furthermore the Purcell factor and the waveguide spectrum results have been shown for the structure with spherical QD in Fig. 13. The electric field of the structure with a spherical QD is the same, with a maximum intensity of 13a.u.

As shown in Figs. 12a and b, the photoluminescence spectrum as well as the Purcell factor fluctuate with the change in wavelength and consecutive peaks are observed. The reason for this oscillating behavior is explained by the change in the emission mode of the emitted photons with the change in wavelength. As the wavelength of the photon emission changes, the emission mode also changes, and the emitter changes phase from the fundamental mode of $HE_{11}$ to higher modes such as $TM_{01}$. Since in single-photon emitter devices based on the excitation of quantum dots within an optical cavity, the goal is to better coupling the photons emitted from the dipole source to the fundamental waveguide mode, so expect the maximum value of the device Purcell factor occurs at the wavelength corresponding to the emission of the $HE_{11}$ mode. As shown in Fig. 12a, the Purcell factor has the highest value in the $HE_{11}$ emission mode at 1024.8 nm. On the other hand, the emission spectrum of the device peaks at the frequencies where the highest value of Purcell factor and the lowest value of cavity losses occur. Observing Fig. 12b, it can be seen that at 1002 nm, the device has the lowest losses and high Purcell factor. Therefore, the highest peak is observed in the device emission spectrum at this wavelength. Other peaks observed are also due to propagation in much higher modes with high Purcell factor.

### Table 1 Characteristics of the final simulated structure

| Characteristics | Dimensions          |
|-----------------|---------------------|
| NW radius       | 220 nm              |
| NW height       | 10 µm               |
| QD radius       | 8 nm                |
| QD shape        | Circle (nano disk)  |
| Z(QD)           | 0                   |

Fig. 11 Final simulated QD within NW structure (dimensions are in nanometers)
Fig. 12  a Purcell spectrum, b PL Spectra of NW waveguide, c Electric field of final structure simulated in FDTD
Fig. 13  a Purcell spectrum, b PL Spectra and c Electric field of NW waveguide; for sphere QD with radius of 8 nm
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values and low losses in the cavity. The concentration of the electric field profile inside the nanowire and around the dipole source shown in Fig. 12c indicates that the electric field is well confined within the optical cavity, and if there is a substrate or an increase in the radius of the nanowire, the field profile restriction to the cavity walls and outside the device is not removed.

4 Conclusion

We have investigated the effect of height and radius of the hexagonal InP nanowire and the location and orientation of dipole source in the Purcell factor and Quality factor. The maximum Purcell factor and Quality factor have obtained for a nanowire with height and radius of 10 μm and 220 nm respectively. We have also observed that for a dipole source which located in the center of the nanowire axis with orientation perpendicular to the axis, we have maximum electric field intensity. Also, the results have shown we have maximum Purcell factor for ∼ 8 nm circular PbS QDs, although they are spherical in practice.

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Declarations

Conflict of interest  There are no conflict of interest to declare.

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