Optimizing the top profile of a nanowire for maximum forward emission*

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(Received 5 May 2011; revised manuscript received 3 June 2011)

The optimal top structure of a nanowire quantum emitter single photon source is significant in improving performance. Based on the axial symmetry of a cylindrical nanowire, this paper optimizes the top profile of a nanowire for the maximum forward emission by combining the geometry projection method and the finite element method. The results indicate that the nanowire with a cambered top has the stronger emission in the forward direction, which is helpful to improve the photon collection efficiency.

Keywords: nanowire, photon collection

PACS: 61.46.Km, 78.67.Uh **DOI:** 10.1088/1674-1056/20/11/116102

1. Introduction

In recent years, semiconductor nanowires have received special attention due to their unique optical and electrical properties.[1−9] The application in single crystalline nanowires made from GaN, ZnO or CdS may play an important role in promoting the optoelectronic technology.[10−14] An important nanowire application is the solid-state sources of single photons (S4Ps), which can be made by embedding a quantum emitter, a quantum dot (QD) for example, in a single model nanowire.[15] The development of efficient S4Ps is now a major challenge in the context of quantum information processing[16] and quantum communications.[17] The optimal design of the nanowire and quantum emitter based S4Ps structure may be one of the key technologies for promoting the collection efficiency of S4Ps.

The collection efficiency is especially sensitive to the top profile of the nanowire. So the research of several groups have been focused on the emission properties of varied nanowires. These include studies on the mode quality factor,[18] the emitting properties of nanowire with hexagonal or circular sections,[19] the far-field emission,[20] control of the emission profile with a conical taper[21] and the design of the nanowire antenna.[22] Very high extraction efficiencies can be obtained by the nanowire with a truncated conical taper.[21,22] However, the design of the nanowire top profile is only parametric optimization. The optimal topology design for the top profile of nanowire may approach the maximum collection efficiency for S4Ps. In this paper, we combine the topology optimization and the parametric optimization to seek the optimal top structure of the nanowire.

The total efficiency of S4Ps is mainly governed by two parameters: the β factor and the extraction efficiency η.[23] The maximum β can be achieved by choosing the suitable nanowire radius[24] and η can be improved by devising the nanowire geometry. The field in the nanowire is superposed by forward and backward propagating guided modes. At the top of nanowire, the mode is partly transmitted into free space and partly reflected back into the nanowire. An efficient bottom of the nanowire is planar metallic mirror, which can reflect guided wave to the front perfectly.[22] In this paper, we assume that the backward field is reflected forward. Thus, to find the optimal top structure of the nanowire, we only consider the guided mode that is injected forward at the bot-

*Project supported by the National High Technology Research and Development Program of China (Grant No. 2009AA03Z405), the National Natural Science Foundation of China (Grant Nos. 60971068, 60908028, and 10979065), the Fundamental Research Funds for the Central Universities of China (Grant No. BUPT2009RC0411), Program for New Century Excellent Talents in University of China (Grant No. NTCE-10-0261), and the Chinese Universities Scientific Fund (Grant No. 2011RC0402).

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tom of nanowire to simplify the model.

In this paper, the geometry projection method (GPM)[25,26] and finite element method (FEM) are combined to optimize the top geometry of the nanowire for improving the collection efficiency of S4Ps. The GPM is used here to reduce the quantity of calculation by introducing the alternative approach for structure optimization. And the FEM is appropriate to compute the emission property of the nanowire with arbitrary dielectric materials distribution. Finally, we use the Nelder-Mead algorithm to search for the optimal top structure of the nanowire for a stronger emission in the forward direction. This work demonstrates a novel way to optimize the nanowire geometry by introducing the axial symmetry of the cylindrical nanowire.

2. Model and methodology

The nanowire structure to be optimized is shown in Fig. 1, it is assumed to be a homogenous material with a refractive index $n = 3.45$ (GaAs) and a radius $r = 105$ nm (for the largest coupling factor β.[22]) A design region is located at the top of the cylindrical nanowire, and a target region with radius $R = 3r$ is away from the design region with $d = 3r$. The heights of the design region and nanowire are 200 nm and 1000 nm respectively. The symmetry of the nanowire structure is exploited in the FEM model to reduce the quantity of calculation, only a quarter of the total structure has to be calculated. A port source is used to excite the fundamental mode HE_{11} at the bottom of the nanowire. A perfectly electrically conducting (PEC) boundary condition is used at the surfaces on the *yoz* plane and a perfectly magnetically conducting (PMC) boundary condition is used at the surfaces on the *xoz* plane (the arrangements of these two boundary conditions correspond to two different polarizations of the fundamental mode HE_{11}). An absorbing boundary condition (ABC) is used at other boundaries to free space. A perfectly matched layer (PML) is adjacent to the ABC's to minimize the spurious reflection.[26]

To achieve accurate results, the refined mesh and second-order isoparametric vector elements are used in the model. The maximum element size in design and target regions is 10 nm, in nanowire region is 20 nm, and other regions are meshed automatically. At least two layers of elememts are required along the absorbing boundary of the PML region, and a minimum of four elements per wavelength is satisfied. The total number of elements is approximately 50000. Although a more refined solution is possible, the solution time will increase with no help for improving the accuracy.

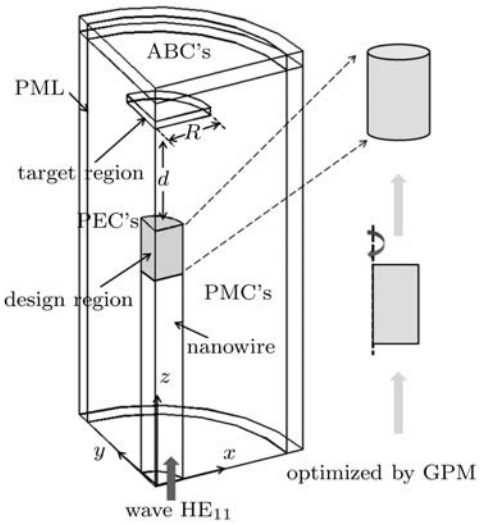


Fig. 1. The finite element model for optimizing the top profile of the nanowire.

Based on the axial symmetry of the cylindrical nanowire, the top profile of the nanowire is optimized by using GPM to reduce the quantity of calculation. As shown in Fig. 2, the essence of GPM is to adjust the shape of the projection by adjusting the shape of the three-dimensional surface $S(x)$. The surface is fitted by a set of the control point which has different heights. The surface function is given by

$$S(x) = c_0 + c \cdot x + \sum_{\mathrm{p}} \lambda_{\mathrm{p}} \Phi(|x - x_{\mathrm{p}}|), \tag{1}$$

$$\Phi(r) = r^2 \lg r, \tag{2}$$

where x and x_{p} are the coordinates of the refined mesh of the design domain and the mesh of the control points, respectively. The details of the fitting method and the coefficients c, c_0 and λ_{p} can be found in Ref. [27]. Then, the distribution of the dielectric materials can be obtained by calculating the projection of the surface to a level plane. The distribution of the dielectric materials can be written as[28]

$$\varepsilon_r(x) = \varepsilon_{r,\min} + \frac{(\varepsilon_{r,\max} - \varepsilon_{r,\min})}{2} \times \left(\tanh \left[\frac{\mathrm{sign}[S(x)] \cdot d(x)}{\xi} \right] + 1 \right), \tag{3}$$

$$d(x) = \min_x |x - x_0|, \tag{4}$$

where x_0 is the coordinate of the intersection curve of a level plane with the surface, the available ξ is set to control the intermediate dielectric vanish, and $d(x)$ is the minimum distance from any point to the nearest intersection curve. We can construct the initial

top profile of the nanowire by giving specific heights to the control points and adjusting those heights will change the top profile.

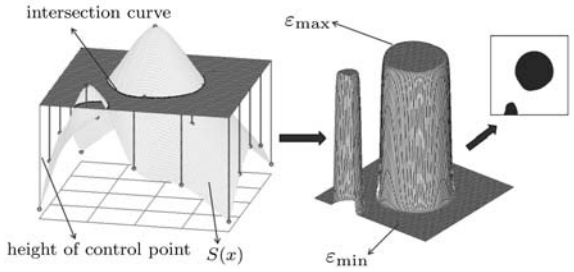


Fig. 2. The schematics of the GPM.

The forward emission performance of the nanowire is quantified by the power flux crossing the target region as shown in Fig. 1. The target function is given by

$$P = \int_{\Gamma} \frac{1}{2}\mathrm{Re}(\boldsymbol{E} \times \boldsymbol{H}^*)\,\mathrm{d}\boldsymbol{s}, \tag{5}$$

where Γ is the bottom boundary of the target region. The design variable is the heights of the control points constructed by the GPM. If we adjust the heights, the geometry of the nanowire top will change. The work in this paper is to optimize the heights of the control points for a maximum forward emission. In order to give an all-round demonstration, we investigate the forward emission pattern as a function of the solid angle, and the function is calculated by

$$S(\theta) = \int_{\Gamma(\theta)} \frac{1}{2}\mathrm{Re}(\boldsymbol{E} \times \boldsymbol{H}^*)\,\mathrm{d}\boldsymbol{s}, \tag{6}$$

$$\Gamma(\theta) = \int_{\theta-0.5\pi/N}^{\theta} R^2\,\mathrm{d}\theta, \tag{7}$$

where $\Gamma\ (\theta)$ means that the one in eight of the spherical surfaces is divided into N equal parts (as shown in Fig. 3, $N = 10$ and $\theta > 0$). The surface integral of the power flux across the spherical surface can exhibit the power distribution from the top of the nanowire.

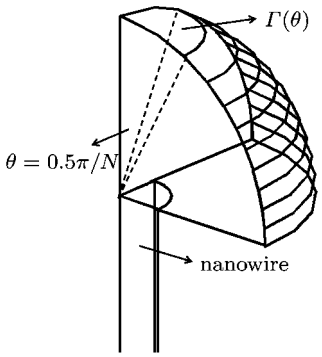


Fig. 3. The spherical surface for the surface integral of the power flux.

3. Results and discussion

In this paper, we optimize the top profile of the cylindrical nanowire with the fundamental mode HE_{11} injected ($\lambda = 0.95$ nm) and choose the radius of nanowire to be around $r = 0.11\lambda$ for the large β value to implement broadband S4Ps.[19] Moreover, we restrict the study to the transmission characteristic of the nanowire top and thus we can neglect the field reflected by the bottom. The simplified model neglects some information, such as the emission property of the embedded QD and the emitter mode coupling. However, the optimization method and the simplified investigation in this paper can still give some useful directions to experiments.

The optimized result is given in Fig. 4. It indicates that the nanowire with the cambered top has the stronger emission in the forward direction, which is helpful to collect photons. However, the emission within an angle of 10° still needs to be improved.

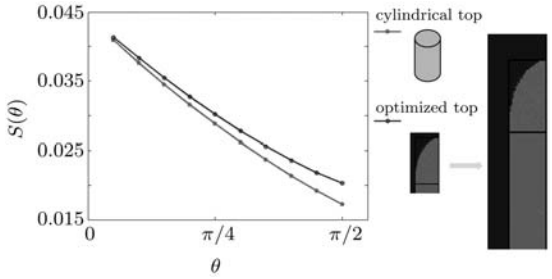


Fig. 4. The forward emission property of the optimized top and the cylindrical top of the nanowire.

Besides the topology optimization, the parametric optimization is also used here to find the optimal structure for the cambered top nanowire. The cambered top is described by a parameter $\alpha = h/r$, where h and r are the height and the radius of the cambered top, respectively. The realationship between α and the value of target function is given in Fig. 5. The study indicated that the cambered top with α around 1.2 has a minimum forward emission and that with α around 3.4 has a maximum forward emission. To find the reasons for this, we study the forward emission property of the cambered top with different α and the results are shown in Fig. 6. When $\alpha < 1$, the emission through the top is predominant and the alternation of α can only influence the emission within an angle of 45°. When $\alpha > 1$, the emission through the slanting side of the cambered top is increased. The maximum forward emission can be obtained by coordinating the emission through the top and slanting side of the cambered top.

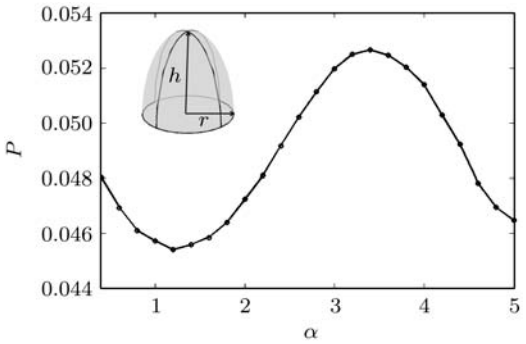


Fig. 5. The target function of the cambered top with different α.

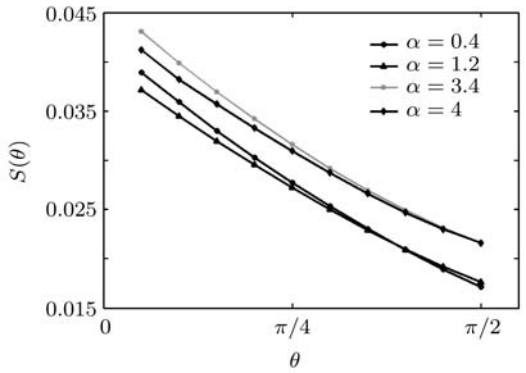


Fig. 6. The forward emission property of the cambered top with different α.

After the topology optimization and the parametric optimization, the forward emission of the cambered top ($\alpha = 3.4$) is obviously stronger than that for a nanowire with cylindrical top (as shown in Fig. 7). We can intuitively understand this by observing the electric field distribution for cylindrical top and the cambered top ($\alpha = 3.4$) as shown in Fig. 8. For a cylindrical top, the forward field is only influenced by the top of the nanowire. The field can be enhanced by the emission through the slanting side of the cambered top. This means that photons are easier to be obtained through the nanowire with cambered top ($\alpha = 3.4$) than that with cylindrical top. So the cambered top is meaningful to the improvement of the photon collection efficiency.

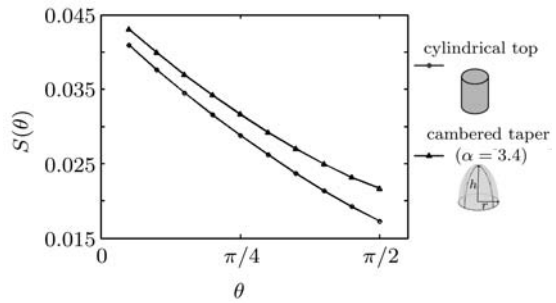


Fig. 7. The forward emission property of the nanowire with different top.

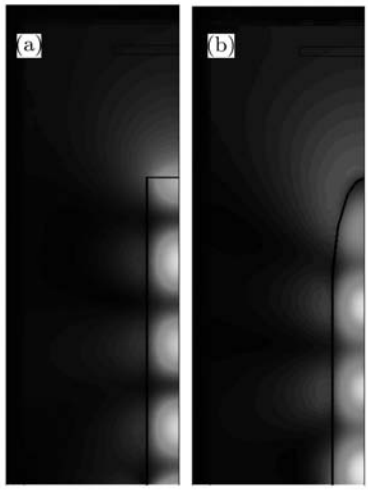


Fig. 8. The electric distribution for nanowire with (a) cylindrical top and (b) cambered top.

In practice, the extraction efficiency of about 17% has been measured in an experiment for a single InAs QD located in a GaAs nanowire, and it is presently limited by photons escaping to the substrate and the large divergence of the forward emission.[24] The model in this paper neglects some important information, such as the surface coarseness of nanowire, the photons reflected by the top of nanowire and the photons escaping from the bottom. It only considers the photons that propagates from bottom to top, and optimize the top profile of the nanowire. The simple theoretical study has demonstrated a way to reduce divergence of the forward emission, which may give some guides to experiments for improving the photon collection efficiency.

4. Conclusion

This paper adopts the GPM and FEM to optimize the top profile of the nanowire for the maximum forward emission. Both topology optimization and parametric optimization are used to seek the optimal top structure of nanowire. The results indicate that the cambered top ($\alpha = 3.4$) has greater potential in improving the photon collection efficiency than the cylindrical top. All the calculations in this paper are based on a simplified FEM model. However, for the problems of back emission, the surface coarseness and the fabrication of nanowire with cambered top are still in need of further research. The study in this paper gives a novel way to optimize the nanowire geometry, which may give some useful directions to the nanowire research.

Acknowledgement

We are grateful to Yao Wen-Jie, Xin Xia for providing us with significant help.

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