Inverse Design for Full Control of Spontaneous Emission Using Light Emitting Scattering Optical Elements

Andreas Håkansson, Hideki T. Miyazaki, and José Sánchez-Dehesa^{1,*}

¹Wave Phenomena Group, Nanophotonics Technology Center, Polytechnic University of Valencia, C/Camino de Vera s/n, E-46022, Valencia, Spain

²Materials Engineering Laboratory, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan (Received 2 January 2006; published 21 April 2006)

Full control of spontaneous emission is essential in various fields of optics. This work presents an inverse designed light-emitting scattering optical element that includes full control of spontaneously emitted photons (i.e., enhancement at a central frequency and suppression at neighboring frequencies) and directionality of the output beam. This is achieved by embedding a one-dimensional optical active element inside a cluster of square shaped gallium arsenide dielectric rods whose positions are optimized by a genetic algorithm. Large spontaneous emission enhancement of >70 is predicted at the transition wavelength if high-quality sources are employed. Moreover, neighboring wavelengths are simultaneously suppressed over 10 times. Finally, the radiated beam is highly collimated to only 6° and contains 30 times the energy emitted by the source placed in free space.

DOI: 10.1103/PhysRevLett.96.153902 PACS numbers: 42.72.Ai, 42.25.Fx, 78.45.+h

The spontaneous emission (SE) of light from a radiating system is highly dependent on its surrounding environment [1]. By controlling the density of photonic states at the transition frequency the SE can be either enhanced or attenuated. This control is fundamental for the performance of various devices in different field of photonics, such as light-emitting diodes, lasers, solar cells, and quantum-information systems. In addition, to increase the functionality of these devices it is essential to control the distribution of the emitted light. In other words, SE that does not contribute to an increase in the device's performance can instead lead to losses or noise.

Photonic crystals [2,3] are predicted to provide high SE control. Recently Fujita *et al.* [4] reported experimental results for redistribution of spontaneous light emission in two-dimensional (2D) photonic crystals following the theoretical work of Fan *et al.* [5]. Though the energy redistribution was positively confirmed, the overall spontaneous emission rate was reduced by a factor of 5 as a result of the 2D photonic band gap effect. However, photonic crystal microcavities show very high SE enhancement due to their small mode volume and high-quality factor (Q) [6–8]. Also, microcavities in planar photonic crystals could be used as single photon on demand sources [9].

This Letter shows that the control of the density and directionality of photons spontaneously emitted from an active source can simultaneously be achieved on a single device using light-emitting (LE) scattering optical elements (SOEs) [10]. SOEs can be seen as extended diffractive optical elements (DOEs) [11] where an additional dimension of design control has been introduced. Instead of the DOEs single layer phase controlling elements, SOEs are based on a few layers of individual constituents whose shape and positions are inverse designed to accomplish a fixed functionality. The SOEs also show great adaptability

to integrate multiple functionalities on a single solid device with dimensions of a few wavelengths. The LE-SOE reported here simultaneously performs enhancement at the transition wavelength, suppression at neighboring wavelengths, and directionality of the light spontaneously emitted by its active component.

The SOE inverse design (ID) tool requires a fast and accurate electromagnetic field simulator and a global optimization method. In accordance with these criteria, a semi-analytical wave expansion method, the multiple scattering theory [12], is applied to solve Maxwell's equation for systems of 2D dielectric rods. This method is very fast when dealing with systems of less than 100 scatterers. They can be simulated in a few seconds using a Pentium IV proces-

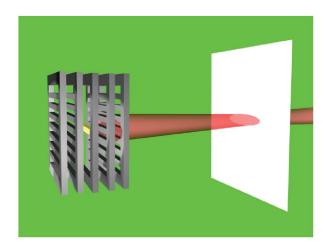


FIG. 1 (color). Schematic view of a light-emitting SOE. An active optical element (yellow rod) is incorporated into the central plate. The red beam illustrates the collimated emitted light. The white plane is an image projection of the emitted light in the far field.

sor. For global optimization a popular stochastic search method is chosen, the genetic algorithm (GA) [13,14], since it has been proven to be effective in finding global optimum of complex problems in photonics [10,15–17].

To run the ID algorithm on a standard personal computer we employ a set of constraints, defined by choosing a specific fabrication method and work within its boundaries. A promising method to fabricate real three-dimensional LE-SOEs consists of stacking individual designed dielectric plates perfectly aligned by using a micromanipulation technique [18,19]. To make 2D structures, parallel rods are etched out from each plate. Furthermore, the central plate incorporates a single rod with an embedded light-emitting quantum wire. A schematic view of the proposed LE-SOE device is illustrated in Fig. 1. Although scaled units will be used throughout this work, the actual proposed source emits light at the wavelength (λ_e) of 1550 nm with a linewidth $(\Delta \lambda_e)$ of roughly 100 nm. The corresponding decay rate $\gamma_e (= \Delta \lambda_e / \lambda_e)$ is equal to 0.064, which is typical value for quantum wires lasing at room temperature. The refractive index of the rods is that of gallium arsenide (GaAs), which at λ_e is 3.4. The position and width of the rods etched out of the plates can be chosen almost freely, but for simplicity, square shaped rods as well as discrete positions are chosen for the LE-SOE design presented here. Even under these constraints, this fabrication method gives a great number of different possible designs that can be manufactured. This large variation is an important part of the ID process.

We look for a LE-SOE device highly increasing the power emission at the transition wavelength of emitter. Furthermore, it should suppress the emission for neighboring wavelengths to get a narrow spectra resulting in a very energy efficient emitter. Finally, it is also desirable that the emitted light at the transition wavelength should be collimated. In other words, the goal of our work is to design a perfect light source.

In order to control the light emission, the density of optical states must be manipulated. Here, the emission from a dipole with an out-of-plane polarization (TM mode) embedded inside a rod will be used as the emitting source. This polarization is dominant for a system incorporating a quantum wire [20].

The electric field distribution for an out-of-plane polarized dipole in free space is $H(kr)e^{-i\phi}$, where H is the Hankel function and k is the wave vector. The multiple scattering theory, as derived in [12], has to be extended to include sources inside scattering objects. This is accomplished by a simple modification of the boundary condition equation. For dielectric rods the boundary continuous conditions from Maxwell's equations are

$$E_{+} = E_{-}, \qquad \hat{n} \cdot (\nabla \cdot E)_{+} = \hat{n} \cdot (\nabla \cdot E)_{-}, \qquad (1)$$

where (+) and (-) correspond to exterior and interior fields, respectively. If a source is placed inside a rod, E_+ and E_- in Eq. (1) are expressed as

$$E_{+} = E_{t}(k_{1}), \qquad E_{-} = E_{s}(k_{2}) + E_{r}(k_{2}), \qquad (2)$$

where E_s , E_r and E_t are the source, reflected, and transmitted waves and k_1 and k_2 are the wave vectors in the background and inside the rods, respectively. Now, it is the transmitted wave (t), and not the scattered wave (s), that is emitted by the rod into the background medium.

The relationship between the three fields in Eq. (2) can be cast into matrix form using the same steps done by Waterman [21,22]. Afterward, the behavior of a source placed inside a scatterer can be analytically expressed using this matrix relation. Here, the emission profile of the TM polarized dipole placed in the center of a square-shaped rod is not changed for rod dimensions much smaller than the wavelength; the wave transmitted though the scatterer, E_t , behaves exactly as a dipole in free space. The rod with the embedded dipole will be treated as the source of our LE-SOE setup.

The active single-rod plate is sandwiched in between eight plates (four at each side), resulting in a total of nine layers SOE device. Even though an increase in layers would likely result in a better performance, the number of plates is intentionally kept low to facilitate the fabrication process. To compare with a heuristic direct-design approach, a 2D high-Q cavity would be very intricate to design since no scatterers can be included in the plate containing the LE rod, which makes it impossible to completely enclose the source. By using our inverse design approach, we are not hindered by any such obstacles.

We here choose to work with fixed size square shaped rods of dimension $a \times a$, placed in fixed lattice sites (LS). The binary design variables simply code the presence or absence of the rods at the fixed LS. The LS are chosen so all rods will be separated from each other; two rods in neighboring plates are never placed exactly atop of one another. This specific limitation is set by the simulation tool since the standard multiple scattering theory cannot deal with close packed structures. More specifically, the LS on each plate are separated a distance of 2.25a, where a is the thickness of the plates. Each plate contains alternating 16 and 17 LS resulting in the a total width of 36a and a total of $4 \times (16 + 17) = 132$ binary parameters. These 132 variables equal $2^{132} \cong 5.44 \times 10^{39}$ different designs. The functionality for each possible LE-SOE designs is estimated by the value taken by a defined fitness function, f. The higher the fitness value the better the functionality. Since the goal is to simultaneously control three different photon emission characteristics, i.e., enhancement (ϵ) , suppression (σ) , and collimation (c), this function was set to

$$f(\vec{s}) = (\epsilon \sigma c^2)^{1/4},\tag{3}$$

where \vec{s} includes the design variables. Parameter ϵ is the reduction of SE lifetime obtained as the ratio between the total energy radiated by the source inside the LE-SOE device and the source in free space [23]. It is calculated at λ_e (= 3.875a for a = 400 nm) and represents the

Purcell factor, a figure of merit of the cavity alone that describes its ability to increase the coupling of an ideal emitter with the vacuum field. To calculate the total energy radiated [23,24], the Poyntyng vector of that radiation field is integrated over a line enclosing the device. Similar calculations are performed for four different transitions wavelengths over a range of 0.25a (100 nm) around λ_e ; i.e., at 3.75a, 3.81a, 3.94a, and 4.00a. The inverse of the arithmetic mean of the four calculated SE modifications is taken as the σ parameter in Eq. (3). Finally, c was evaluated as the amplitude of the electric field in a far-field point located at the positive x axis of the SOE. The square of the c variable in the fitness equation was set to emphasize the collimation and the 1/4 exponent is only included to adjust the scale.

Figure 2 shows the performance of the ID designed device found by the GA maximizing the fitness in Eq. (3). Both the far field [Fig. 2(a)] and near field [Fig. 2(b)] of the scattered electric field produced by the embedded source for the central wavelength λ_e are represented. Also, the collimation can be observed in Fig. 2(a), where the modulus of the electric field amplitude is plotted for a large area surrounding the device. Figure 2(b) depicts the real part of the electric field inside the LE-SOE as well as the position of the individual rods, which are defined by the white squares. The localized optical mode, which is observed at the center of this LE-SOE, has it maximum intensity at the position of the central rod (the active component in this device).

Now, let us discuss in brief how the density of photons emitted is modified in this device. The reduction of the SE

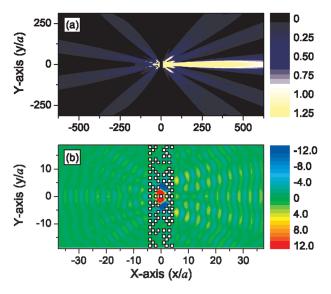


FIG. 2 (color). Performance of the optimized LE-SOE device at the central wavelength of the emitting source. (a) Amplitude of the electric field showing the collimation of light emission in the far field. (b) The real part of the electric field in near field. The white squares represent the position of GaAs rods in the LE-SOE device. The unit length, a, in both figures represents the thickness of the plates proposed in the fabrication method.

lifetime (τ) for an emitter in a resonant cavity is derived directly from the rate (Γ) given by Fermi's golden rule:

$$\frac{1}{\tau} = \frac{\Gamma}{\hbar} = \frac{2\pi}{\hbar^3} \int_{-\infty}^{\infty} \langle |\vec{p}_{\alpha} \cdot \alpha \vec{E}(\vec{r}_e)|^2 \rangle \rho_c(\omega) \rho_e(\omega) d\omega, \quad (4)$$

where $\rho_c(\omega)$ is the density of photon modes in the cavity, $\rho_e(\omega)$ is the mode density for the dipole transition, \vec{p}_{α} is the atomic dipole momentum, and $\vec{E}(\vec{r}_e)$ is the electric field at the location of the emitter normalized by a factor $\alpha^2 \equiv$

 $\frac{2\pi}{\hbar^2} \frac{4\pi}{\int \epsilon(\vec{r})\vec{E}(\vec{r})^2 d^3r}$ to the zero point energy. For a deltalike emitter of frequency ω' and zero linewidth, $\rho_e(\omega) = \delta(\omega')$, the SE rate is:

$$\Gamma' = \frac{2\pi}{\hbar^2} \langle |\vec{p}_{\alpha} \cdot \alpha \vec{E}(\vec{r}_e)|^2 \rangle_{\omega'} \rho_c(\omega'). \tag{5}$$

As mentioned before, the SE rate can be extracted classically from the dipole radiation power [23]. Therefore, the density of photon modes in the cavity of our LE-SOE can easily be explored in the frequency range of the actual emitter by calculating the SE modification (= Γ'/Γ_0) of various ideal emitters whose frequency is tuned in the range $\omega_e - \frac{\Delta \omega_e}{2} \leq \omega' \leq \omega_e + \frac{\Delta \omega_e}{2}$.

Figure 3 represents the characterization of the cavity alone, depicting the SE modification ability for wavelengths around λ_e . The SE enhancement for λ_e is 72 times the emission of only the central emitting layer. This value defines the Purcell factor of an ideal source ($\gamma_e = 0$) emitting at λ_e . This figure also shows that neighboring wavelengths are suppressed over 10 times. Here the Q value ($=\lambda_e/\Delta\lambda_e'$) is calculated by estimating the peak's width at its half maximum. This predicts an in-plane Q value of approximately 600.

The multiple scattering theory can also be employed to calculate the complex resonance energies of dielectric clusters from which it is possible to analytically extract the optical confined modes (λ_c) and their in-plane O_c

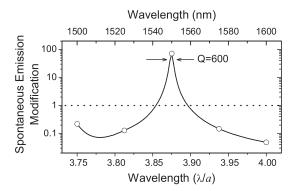


FIG. 3. Spontaneous emission modification for ideal emitters (of deltalike distribution and zero linewidth) having wavelengths within the spectral range used in the design process. The white circles define the five wavelengths incorporated in the optimization process. The Q- value is obtained at the peak half maximum.

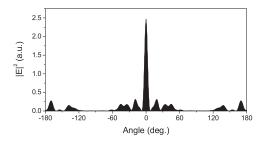


FIG. 4. Angular dependence of the square of the electric field calculated at a radius of 250a from the center of the optimized LE-SOE (see Fig. 2).

value. The possible modes are given by the zeros of the matrix determinant resulting from multiple scattering when no incident wave is assumed [25]. This procedure was applied to calculate the actual parameters of the optical mode for the device shown in Fig. 2(b). The resulting resonant complex wavelength is $\lambda_c = 3.87a - i4612a$ $(=1.549 \mu m - i1844 \mu m)$. Note that the device found by the ID process has its optical resonance—defined by the real part of λ_c —perfectly tuned to the wavelength, λ_e , employed in the optimization. This result is achieved with very few set limitations on the fabrication process. Using the relation $Q_c = -\text{Im}(\lambda_c)/2\text{Re}(\lambda_c)$, the in-plane Q_c takes the value of 595, which is in agreement with the Q calculated in Fig. 3. Though this Q_c value is modest, please note that Q_c is only used for characterization purposes and it is not directly incorporated into the performance evaluation of the LE-SOE.

The LE-SOE is further characterized in Fig. 4 that shows the square of the electric field amplitude in the far field for different angles. The estimated beam's thickness at half power is only 6°. Furthermore, the total radiated energy of the central lobe, spanning from -7.5° to 7.5° , equals 41% of the total energy radiated by the LE-SOE or $0.41 \times 72 = 30$ times the energy emitted by the source placed in free space. This directivity of the LE-SOE has many similarities to the commonly used Yagi-Uda antenna.

The SE enhancement (E) at λ_e with respect to the homogeneous medium has been calculated using the expression obtained in the limit of weak coupling to the cavity mode [24]. Under the assumption of no polarization mismatch $(\eta=1)$ and taking into account the effect of finite decay rates of emitter $(\gamma_e\approx 0.064)$ and cavity mode $(\gamma_c\approx 0.002)$, $E\approx 1.1$. In actual three-dimensional devices, this value could be increased by a strong confinement of the light in the vertical direction and by considering a larger number of layers in the design process.

In conclusion, it has been demonstrated that by using inverse design one can achieve total control of spontaneous light emission. Furthermore, the design process is carried out under the limitations of a fixed fabrication method and with very few constraints. In particular, it has been shown how the emitted light from a dipole can be controlled in the plane by embedding the source in an array of scatterers and

so simultaneously controlling enhancement, suppression, and directionality of spontaneous light emission. We believe that this demonstration is an important step in various fields of photonics of such as, lasers, LEDs, quantum-information systems, and solar cells. Also, since the ID method could be improved along with fabrication method, many constraints could be removed and we will have more freedom of design that will result in an increase of the asked for performance of the optimal design.

The authors acknowledge P. Sanchis for confirming our calculations using a FDTD software package, as well as K. Aoki, Y. Kurokawa, and H. Akiyama for their helpful support. The financial support provided by the Spanish Ministry of Education and Science (Contracts No. TEC2004-02345 and No. NAN2004-08843) and the Japanese Society of Promotion of Science are also gratefully acknowledged.

- *Corresponding author.
- Email address: jsdehesa@upvnet.upv.es
- [1] E. M. Purcell, Phys. Rev. 69, 681 (1946).
- [2] S. John, Phys. Rev. Lett. 58, 2486 (1987).
- [3] E. Yablonovich, Phys. Rev. Lett. 58, 2059 (1987).
- [4] M. Fujita et al., Science 308, 1296 (2005).
- [5] S. Fan, P.R. Villeneuve, and J.D. Joannopoulos, Phys. Rev. Lett. 78, 3294 (1997).
- [6] O. Painter et al., Science 284, 1819 (1999).
- [7] Y. Akahane et al., Nature (London) 425, 944 (2003).
- [8] J. Hwang, H. Ryu, and Y. Lee, Phys. Rev. B 60, 4688 (1999).
- [9] P. Michler et al., Science 290, 2282 (2000).
- [10] A. Håkansson and J. Sánchez-Dehesa, Appl. Phys. Lett. 87, 193506 (2005).
- [11] J. L. Horner and P. D. Gianino, Appl. Opt. 23, 812 (1984).
- [12] A. Ishimaru, Electromagnetic Wave Propagation, Radiation, and Scattering (Prentice Hall, Englewood Cliffs, NJ, 1991).
- [13] J. H. Holland, *Adaptation in Natural and Artificial Systems* (The University of Michigan Press, Ann Arbor, 1975).
- [14] D. Goldberg, Genetic Algorithms in Search, Optimization and Learning (Addison-Wesley, Reading, MA, 1989).
- [15] M. M Spuhler *et al.*, J. Lightwave Technol. **16**, 1680 (1998).
- [16] L. Sanchis et al., Appl. Phys. Lett. 84, 4460 (2004).
- [17] S. Preble, M. Lipson, and H. Lipson, Appl. Phys. Lett. 86, 061111 (2005).
- [18] K. Aoki et al., Nat. Mater. 2, 117 (2003).
- [19] K. Aoki et al., Appl. Phys. Lett. 81, 3122 (2002).
- [20] L. A. Coldren and S. W. Corzine, *Diode Lasers and Photonic Integrated Circuits* (Wiley-Interscience Publication, New York, 1995).
- [21] P.C. Waterman, J. Opt. Soc. Am. A 16, 2968 (1999).
- [22] P.C. Waterman, Phys. Rev. D 3, 825 (1971).
- [23] Y. Xu et al., J. Opt. Soc. Am. B 16, 465 (1999).
- [24] H. Y. Ryu and M. Notomi, Opt. Lett. 28, 2390 (2003).
- [25] S. Nojima, Appl. Phys. Lett. **79**, 1959 (2001).