Effective mode area and its optimization in silicon-nanocrystal waveguides

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We revisit the problem of the optimization of a silicon-nanocrystal (Si-NC) waveguide, aiming to attain the maximum field confinement inside its nonlinear core and to ensure optimal waveguide performance for a given mode power. Using a Si-NC/SiO_2 slot waveguide as an example, we show that the common definition of the effective mode area may lead to significant errors in estimation of optical intensity governing the nonlinear optical response and, as a result, to poor strength evaluation of the associated nonlinear effects. A simple and physically meaningful definition of the effective mode area is given to relate the total mode power to the average field intensity inside the nonlinear region and is employed to study the optimal parameters of Si-NC slot waveguides.

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Silica (SiO_2) embedded with silicon nanocrystals (Si-NCs) is considered a promising nonlinear material, as it exhibits a strong ultrafast Kerr effect and can also be used with the current complementary metal–oxide–semiconductor technologies [1–3]. These features make the Si-NC/SiO_2 composite especially attractive for ultrafast all-optical switching and modulation, and recent experiments demonstrate that bit rates beyond 100 Gb/s are feasible [2]. Because of its relatively low refractive index, this composite material is unable to confine light tightly enough to meet the miniaturization demands of modern photonics nanocircuitry. However, it can be used as an active medium within plasmonic or dielectric waveguides, designed with high index contrasts and providing strong field confinement required for the nonlinear effects to occur at moderate power levels. The strength of any nonlinear phenomenon is determined by the intensity of light inside the nonlinear medium, which is related to the mode power through the effective mode area (EMA) [4]. Unfortunately, the absence of a unique definition for the EMA has recently led to confusion in the optimization of the nonlinear performance of Si-NC/SiO_2 waveguides, associated with the employment of an inappropriate definition [5]. In this letter, we clarify this issue and revisit the problem of the nonlinear performance assessment.

The effective area A_{eff} of a guided mode, characterized by the electric field $\mathbf{E}(x,y)$ and the magnetic field $\mathbf{H}(x,y)$, is introduced naturally during the derivation of the nonlinear Schrödinger equation (NLSE) [6]. If such a derivation takes into account the full vectorial nature of the electromagnetic field, the resulting definition is [7]

$$A_{\mathrm{eff}} = \left(\iint_{-\infty}^{\infty} S_z \mathrm{d}x\mathrm{d}y\right)^2 \Big/ \iint_{-\infty}^{\infty} S_z^2 \mathrm{d}x\mathrm{d}y, \qquad (1)$$

where $S_z = (\mathbf{E}\times\mathbf{H})\cdot\hat{z}$ is the time-averaged z component of the Poynting vector, $\hat{z}$ is the unit vector along the waveguide axis, and the integration is over the entire $x-y$ plane. In the weak-guidance approximation, implying that the refractive index varies slowly in the transverse direction, this definition leads to the well-known expression [4,6,8]

$$A_{\mathrm{eff}} = \left(\iint_{-\infty}^{\infty} |F(x,y)|^2 \mathrm{d}x\mathrm{d}y\right)^2 \Big/ \iint_{-\infty}^{\infty} |F(x,y)|^4 \mathrm{d}x\mathrm{d}y, \qquad (2)$$

in which the lateral field profile is represented by a single scalar function $F(x,y)$.

Of primary importance for a nonlinear waveguide is the average field intensity I_{NL} inside its nonlinear constituent, as it determines the efficiency of all nonlinear effects developing inside the waveguide. Without loss of generality, we focus on a quasi-TM mode with the dominant component of the electric field being in the x direction (so that $F \approx E_x$). It turns out after some reflection that neither Eq. (1) nor Eq. (2) can be used to relate I_{NL} to the total power P of this mode, as none of them explicitly contains the lateral dimensions of the waveguide. The equality $I_{\mathrm{NL}} = P/A_{\mathrm{eff}}$ would hold only if S_z (or E_x) was uniform inside the nonlinear region and zero outside of it, in which case A_{eff} is simply equal to the region's cross-section area a_{NL}.

It is not hard to construct a proper factor relating P and I_{NL}, and we introduce a new EMA in the form

$$a_{\mathrm{eff}} = a_{\mathrm{NL}} \iint_{-\infty}^{\infty} S_z \mathrm{d}x\mathrm{d}y \Big/ \iint_{\mathrm{NL}} S_z \mathrm{d}x\mathrm{d}y, \qquad (3)$$

where NL denotes integration over the nonlinear region. Since the surface integrals in this expression give the total mode power (numerator) and the power P_{NL} transmitted through the nonlinear part of the waveguide (denominator), we can write $I_{\mathrm{NL}} = P_{\mathrm{NL}}/a_{\mathrm{NL}} = P/a_{\mathrm{eff}}$. Hence, while the effective area given in Eq. (1) or Eq. (2) determines the relative efficiency of the nonlinear effects within the framework of the NLSE, the quantity in Eq. (3) allows one to estimate the actual intensity of light inside the nonlinear waveguide. These equations are inapplicable to plasmonic waveguides, where S_z has different signs inside metal and dielectric, and thus the total power flow may vanish.

To better understand the difference between the preceding definitions, consider an optical fiber with a highly nonlinear core (e.g., a silicon-core fiber) and assume that

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the Poynting vector decays with distance r from its axis as $S_z \propto \exp(-r^2/w^2)$, where w is the mode-size parameter. In this case, Eqs. (1) and (3) give $A_{\text{eff}} = 2\pi w^2$ and $a_{\text{eff}} = \pi w_{\text{NL}}^2[1 - \exp(-\xi^2)]^{-1}$, where w_{NL} is the radius of the nonlinear core and $\xi = w_{\text{NL}}/w$ is the confinement factor. If the mode extends far beyond the nonlinear core ($\xi \ll 1$), values of the two effective areas differ by a factor of 2. In the opposite limit of strong mode confinement with the mode power predominantly residing within the core ($\xi \gg 1$), Eq. (3) gives an adequate result of $a_{\text{eff}} \approx \pi w_{\text{NL}}^2$, whereas Eq. (1) leads to a much larger value ($A_{\text{eff}} \gg \pi w_{\text{NL}}^2$), which is obviously incorrect for the estimation of I_{NL}. This example shows that Eqs. (1) and (2) are unsuitable for evaluating the nonlinear performance of optical waveguides in which the nonlinear effects are dominant within a separate layer of suitable material (such as a Si-NC/SiO_2 waveguide).

As we mentioned earlier, owing to certain arbitrariness in defining EMA, a number of alternative expressions for it may be found in literature [5,9,10]. For instance, Sanchis *et al.* [5] define A_{eff} similar to Eq. (2), but with integrals in the denominator evaluated over the nonlinear region [as in Eq. (3)]. Foster *et al.* [10], on the other hand, employ a definition somewhat similar to that of a_{eff},

$$A_{\text{eff}} = \pi \iint_{-\infty}^{\infty} S_z(x^2 + y^2)\mathrm{d}x\mathrm{d}y \Big/ \iint_{-\infty}^{\infty} S_z \mathrm{d}x\mathrm{d}y,$$

resulting in $A_{\text{eff}} = \pi w^2$ for the earlier example. While Foster *et al.* do recognize that the smallest A_{eff} does not necessarily correspond to the optimal nonlinear performance of the waveguide, Sanchis *et al.* do not. Indeed, they proceed to use their definition for optimizing the nonlinear effects (even though its use leads to wrong conclusions in our opinion).

We now focus on a Si-NC-based slot waveguide shown in Fig. 1(a) and investigate the behavior of different EMAs at the telecom wavelength of 1.55 μm by varying geometric and material parameters of the waveguide. The localization of the optical field inside a highly nonlinear, yet weakly guiding, Si-NC/SiO_2 layer of thickness t is achieved by embedding it between two equally thick layers of silicon ($n_{\text{Si}} = 3.48$) and surrounding the entire ridge of width w with air. The overall structure is fabricated on a silica substrate ($n_{SiO_2} = 1.45$), whose thickness ($H = 0.3$ μm) and width ($W = 1.4$ μm) are assumed to be fixed. The refractive index of the active slot region depends on the excess of silicon in SiO_2, which is determined by the volume fraction f of Si-NCs, and is given by Bruggeman's formula $n_{\text{NC}} = \left\{u + \left[u^2 + \frac{1}{2}(n_{\text{Si}} n_{SiO_2})^2\right]^{1/2}\right\}^{1/2}$, where $u = \frac{1}{4}\left[(2 - 3f)n_{SiO_2}^2 + (3f - 1)n_{\text{Si}}^2\right]$.

Figure 1(b) shows EMAs as functions of waveguide width, calculated from Eqs. (1)–(3) for $h = 500$ nm and 700 nm using COMSOL software with $f = 0.1$ ($n_{\text{NC}} \approx 1.6$) and $t = 100$ nm. As might have been expected based on the analytical example, the three definitions lead to significantly different values of EMA. Relative proximity of the curves obtained from Eqs. (2) and (3) for $h = 500$ nm is a mere coincidence (compare these curves for the thicker waveguide). The minimum value

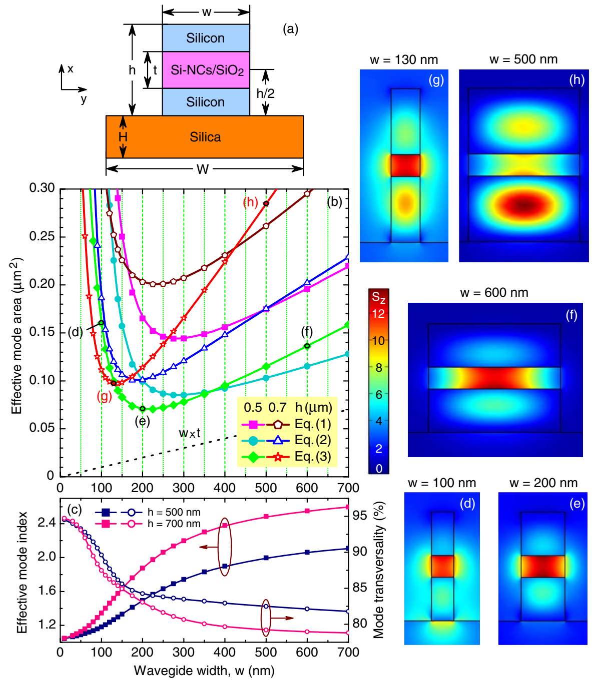

Fig. 1. (Color online) (a) Si-NC/SiO_2 slot waveguide, (b) three types of EMAs, and (c) effective index and transversality of the fundamental quasi-TM mode as functions of waveguide width for 500 and 700 nm thick waveguides. Density plots of Poynting vector in (d)–(h) correspond to locations marked in (b). In all cases, $f = 0.1$ and $t = 100$ nm. For other parameters, refer to the text.

of $a_{\text{eff}} \approx 0.07$ μm^2 [point (e)] is attained for $w \approx 200$ nm and corresponds to the strongest confinement of the mode power inside the gap [see Fig. 1(e)]. If w is decreased, the power flow partially shifts from the gap to the interface between the lower silicon cladding and the substrate, as indicated by Fig. 1(d). In contrast, a_{eff} starts to grow when w is increased either because of the decay of S_z away from the mode center along the y axis [see Fig. 1(f)] or because of the mode capture by the lower cladding [see Fig. 1(h)].

By looking at Fig. 1(b), we also notice that the difference between EMAs obtained from Eqs. (1) and (2) varies with the width of the waveguide. This variation is commonly attributed to the change in mode transversality defined as [7]

$$\tau = \iint_{-\infty}^{\infty} (|E_x|^2 + |E_y|^2)\mathrm{d}x\mathrm{d}y \Big/ \iint_{-\infty}^{\infty} |\mathbf{E}|^2 \mathrm{d}x\mathrm{d}y, \quad (4)$$

where in calculating $|\mathbf{E}|^2$ it should be taken into account that E_z is out of phase with E_x and E_y. The transversality and effective index (n_{eff}) of the quasi-TM mode are shown in Fig. 1(c). In the range 150 nm $< w <$ 700 nm, the fractional difference between the two EMAs grows with τ from 30% to 53% for the thicker waveguide and stays around 40% for the thinner one. Such high values are because of the relatively low mode transversality, $\tau \approx$ 79%–85%. As w is decreased to 50 nm and τ exceeds 93%, the difference steeply drops below 10% and n_{eff} becomes close to unity, indicating weak mode guidance and its predominant propagation through air.

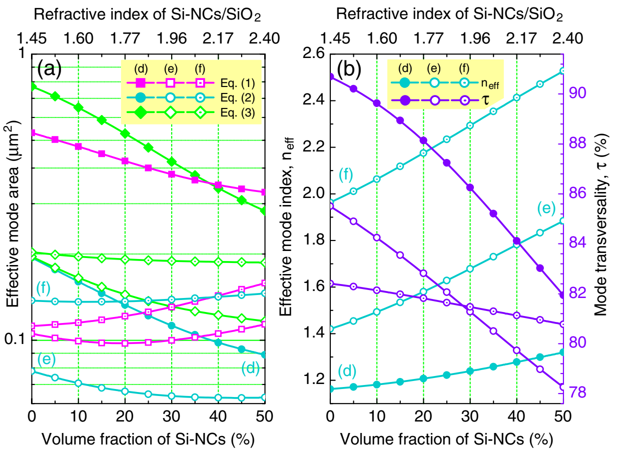

Fig. 2. (Color online) (a) Effective mode area, (b) effective mode index and transversality as functions of Si-NC fraction f in the slot region for three waveguides corresponding to points (d), (e), and (f) in Fig. 1(b). Upper scales show the effective refractive index of Si-NC/SiO_2 composite. Material parameters are the same as in Fig. 1.

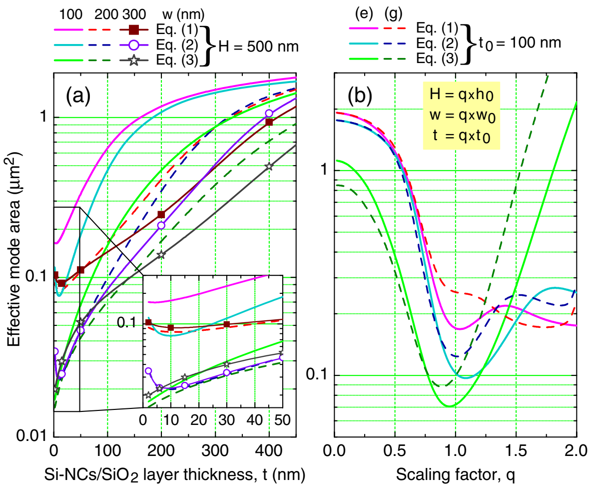

Fig. 3. (Color online) Effective mode area versus (a) thickness of Si-NC/SiO_2 layer and (b) scaling factor q for $f = 0.1$. Legends above the panels show waveguide dimensions and equations employed. Two sets of curves in (b) correspond to optimum waveguide parameters in Fig. 1(e): $h_0 = 500$ nm, $w_0 = 200$ nm, $t_0 = 100$ nm; and in Fig. 1(g): $h_0 = 700$ nm, $w_0 = 130$ nm, $t_0 = 100$ nm. For other parameters, refer to the text.

The refractive index of Si-NC/SiO_2 medium may be tuned over a sufficiently broad range by changing the density of Si-NCs (through silicon excess in the SiO_x composite) before its annealing [2]. Figure 2 shows how such tuning affects different mode parameters for the three waveguides in Figs. 1(d)–1(f). It is seen that the EMAs and mode transversality become more sensitive to changes in volume fraction f of Si-NCs as the waveguide becomes narrower. This behavior is in sharp contrast to that of n_{eff}, which grows faster with f in wider waveguides. Although a_{eff} may be minimized with respect to the parameter f, the optimal performance of the waveguide is not determined by this minimum, because the efficiency of a nonlinear process directly depends on the concentration of Si-NCs. Also noteworthy is that the difference between EMAs calculated with Eqs. (1) and (2) is no longer governed by τ if mode transversality is relatively small [as it occurs for Fig. 1(f)].

Figure 3(a) shows the impact of slot thickness t on EMAs. As seen there, EMAs become especially small when the slot becomes narrower than 100 nm. For instance, when $t = 30$ nm (about ten times larger than the diameter of a typical nanocrystal) and $w = 200$ nm, we obtain $a_{eff} \approx 0.03\ \mu m^2$. The use of Eq. (1) in this case would lead to a threefold underestimation of light intensity for a given mode power. To make the waveguide more compact, one may opt to scale down its optimal dimensions h_0, w_0, and t_0, while keeping their aspect ratio fixed. As Fig. 3(b) suggests, the scaling factor q is a crucial parameter, and halving optimal dimensions may enlarge a_{eff} by more than five times. When q approaches zero, EMAs tend to finite values rather than diverging, as in Fig. 1(b), where only w was reduced.

In summary, we have studied the optimization problem for Si-NC/SiO_2 waveguides by introducing a new definition for its EMA, which relates the total mode power to the average field intensity responsible for the strength of the nonlinear interaction. The new definition was compared to the common ones for different geometric and material parameters of a Si-NC-based slot waveguide, revealing significant discrepancies in predictions of its nonlinear performance.

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