Bound state in the continuum in the one-dimensional photonic crystal slab

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Abstract. In this work we developed a design of one-dimensional Si/SiO2 photonic crystal slab supporting so called optical bound states in the continuum – infinitely high-Q optical states with energies lying above the light line of the surrounding space. Such high-Q states are very perspective for many potential applications ranging from on-chip photonics and optical communications to biological sensing and photovoltaics.

1. Introduction

Localization of light in cavities (waveguides) implies that there is no coupling of cavity modes with modes of free space forming a continuum spectrum. Eigenstates of optical systems is localized only if their energies lie under the light line of the surrounding space. Any modes with energies lying in the continuum spectrum (leaky modes) have low quality factor because of the radiation losses. As a result, they have not found wide implementation. However, in 1929 von Neumann and Wigner proposed that the single-particle Schrodinger equation may possesses spatially localized states with energy lying above the asymptotic limit of the potential [1]. For optics, it means existence of localized states with energies from the continuum spectrum of leaky modes. Such states are called bound states in the continuum (BIC).

Marinica et al, following the results by von Neumann and Wigner, proposed the existence of infinitely high-Q (non-radiative) optical states with energies lying above the light line of the surrounding space [2]. As well as in the case considered by von Neumann and Wigner, radiation of optical BIC into the surrounding space disappeared because of the destructive interference. Theory of BIC is actively developed now. Nature of BIC can be explained by interference effects [3], in terms of topological charge [4], or by symmetry properties of eigenmodes and photonic structures [4,5]. First experimental observation of optical BIC was carried out by Plotnik et al in 2011 [6]. Nowadays a lot of scientific groups worldwide investigate the potential applications of BIC in various fields of science and technology [5,7]. Nevertheless, the majority works are theoretical [2-4, 8, 9].

In this work we theoretically analyzed CMOS-compatible one-dimensional photonic structure based on silicon-on-insulator wafer with optical BIC at telecommunication wavelengths (1.5-1.6 microns).

2. Results and discussion

The photonic structure under consideration is shown in the figure 1(a). It consists of rectangular bars with a period a, width w and height t. We propose that the bars are made of crystalline silicon with refractive index about 3.47 surrounded by fused silica with refractive index 1.44. The periodic
geometry results in photonic band structure. The photonic slab supports guided and leaky modes with frequencies embedded in the continuum modes of free space. Leaky resonances have a finite lifetime, however, in the vicinity of specific points the lifetime tends to infinity. These points correspond to BIC.

We consider two types of slabs with fixed ratio of the width \( w \) to the period \( a \): \( w=0.45a \) and \( w=0.5a \). Here we focus on the lowest TE-like mode (electric field lies along bars). The dependence of frequency and Q-factor for this mode on the Bloch wavenumber are shown in figure 1(b, c). Mode structure of the photonic crystal slab was simulated using the finite-element method in Comsol Multiphysics software. The eigenvalue solver returns complex eigenfrequencies \( f \), so it is possible to calculate radiative Q-factor as

\[
Q_r = \frac{\text{Re}(f)}{\text{Im}(f)}.
\]

\[ (1) \]

Figure 1. (a) Design of a photonic crystal slab with one-dimensional periodicity in x-direction and is infinite along y-direction. (b) Calculated band structure for photonic slab with width \( w=0.45a \) and thickness \( t=1.2a \). Cross symbols indicate embedded eigenstates (BIC). (c) Calculated radiative lifetime, that is quality factor of photonic slab. At the certain \( k \) points leaky resonance does not decay and light becomes perfectly confined in the slab. (d), (e) Electric field profile \( E_y \) of the trapped state at zero and nonzero wave vector \( k_x \) respectively, plotted on the \( y=0 \) slice.

One can see that at some \( k \) points lifetime tends to infinity and light becomes perfectly confined in the slab. At these points leaky resonances turn into localized eigenmodes that do not decay. Sometimes eigenvalues existed within light cone, where there is continuum of radiation modes, are called embedded eigenvalues [3].

We discovered that for the photonic crystal slabs with \( w=0.45a \) two BIC may occur (see figure 1). The first one has zero wave vector (\( \Gamma \)-point) that corresponds to the normal incidence of the exciting wave, and the second one has a nonzero wave vector that corresponds to an oblique incidence of the exciting wave. Figure 2 shows the dependence of eigenfrequency at both zero and nonzero \( x \)-component of wave vector from photonic structure design. The second BIC emerges at certain \( t/a \) value. As \( t/a \) increases, the incident angle becomes bigger till it reaches value 90° from air, see figure 3.
In contrast to structures discussed above, photonic crystal slabs with $w=0.5a$ have embedded states at the $\Gamma$ point only.

Both resonances ($\Gamma$ and off-$\Gamma$ BICs) can be tuned to the telecommunication frequency range (1.5 to 1.6 microns) by proper choice of the geometrical parameters of the sample ($w, t, a$). As soon as figure 2 is plotted in terms of dimensionless parameters, it describes any photonic crystal slab specified design. As an example, let us consider the structures with thickness $t=600$ nm, for which figure 4 illustrates results. The frequency range of interest determines the rest geometric parameters ($w, a$).

As an example, we consider the structures with thickness $t=600$ nm. Figure 4 shows the dependence of BIC frequency on the period of the structure for different ratio $w/a$. So, one can see from figure 4 that in order to BIC frequency lies in the telecommunication frequency range the rest
parameters of the structure could be taken, for example, as follows: period $a=500$ nm and width $w=225$ nm.

For these parameters, the first resonance (at the normal incidence) corresponds to 238 THz (1.260 microns) and the second one (at the angle of incidence about 34.3 degrees from air) corresponds to 201 THz (1.491 microns). One can see that the second resonance is close enough to telecommunication wavelength range.

**Figure 5.** Calculated reflectance spectrum: map and cross sections. An incident angle is measured in SiO$_2$ medium. Disappearance of the response around $0^\circ$ and $34.1^\circ$ indicates a trapped state with no leakage.
To confirm existence of BIC we simulated the reflection spectra from the structure under consideration for different angles of incidence. The interference of incident light with leaky modes results in appearance of Fano-type resonances in the reflectance spectra [10]. We observed them nearby the frequencies corresponding to position BIC obtained within the simulation of the mode structure (figure 5). In contrast, perfect BIC has no response in reflection spectrum, because it is decoupled from free space waves. So, disappearance of the response around 0° and 34.1° indicates a trapped state with no leakage.

To summarize, we observed two types of photonic crystal slabs and found out that there are two BICs for slabs with width w=0.45a only. The eigenfrequencies, Q-factors and reflection spectra were calculated. The photonic structures with the proposed design can be fabricated using standard CMOS-compatible silicon-on-insulator wafers.

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