Effect of finite lateral size of dielectric grating on optical bound state in the continuum

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Abstract. Optical bound states in the continuum (BIC) are localized states with energy lying above the light line and having infinite lifetime. Any losses taking place in real systems result in transformation of the bound states into resonant states with finite lifetime. In this work, we analyze properties of BIC in CMOS-compatible one-dimensional photonic structure based on silicon-on-insulator and silicon nitride wafers. We reveal that finite lateral size of samples could destroy both off-Γ BIC and at-Γ BIC turning them into resonant states due to in-plane symmetry breaking.

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, i.e. there is no leakage losses. It follows from the Maxwell’s equations straightforwardly that energies of localized states lie under the light line of the surrounding space. Optical bound states in the continuum (BICs) are a remarkable exception for this general rule. The BICs are spatially bounded (localized in one, two or even three dimensions [1, 2]) eigenstates of an optical system with quality factor that could, in principle, approach infinity despite lying within the light cone of the surrounding space, i.e. in the continuum spectrum of radiative modes. The concept of BIC was firstly proposed by von Neumann and Wigner in 1929 for electron placed in a specific potential [3]. More recently, another examples of electronic BICs have been predicted theoretically in atomic and molecular systems [4] and in artificial systems [5]. In optics, the term bound state in the continuum first appeared around 2008 [6] although this phenomenon has been studied earlier [7]. Experimental observation of optical BIC followed only in 2011 [8].

The main advantage of the bound optical states is the high quality factor which can be of the order of 10^7 and is limited only by the losses in the material and by the roughness of the photonic structures [9]. High quality, CMOS-compatibility and simplicity of geometry and design make the resonators based on the optical bound states in the continuum attractive for wide range of applications beginning with lasers and sensors and ending with nonlinear optical devices.

The next significant feature is feasibility to excite the bound optical states lying inside the light cone by an ordinary plane electromagnetic wave without using any auxiliary devices or tricks such as prisms, diffraction gratings or surface irregularities which are necessary to excite the states outside the light cone. This advantage offers great possibilities of technical applications.

In theory, BICs have infinite high quality factor, however, for real systems it is limited because of material absorption, technological imperfections, roughness, finite lateral size of samples and...
leakage into the substrate. Here, we analyze influence of the finite lateral size on frequency and Q-factor of BICs.

![Figure 1](image.png)

**Figure 1.** (a) Schematic image of a sample. (b) Electric field $|E_y|$ distribution for TE-like mode $E \sim |E_y|e^{-ik_xx}$.

### 2. Results and Discussion

The design of the photonic structure under study is shown in Fig. 1(a). It consists of rectangular bars made of crystalline silicon or silicon nitride surrounded by fused silica. Since the array is periodic in the x-direction, the eigenstates of the structure are characterized by the frequency $f$, the wave vector along the bars $k_y$ and by the Bloch quasi-wave vector $k_x$ restricted to the first Brillouin zone. It has been shown that such one-dimensional photonic structures supports BICs either if wave vector $k_y$ or quasi-wave vector $k_x$ is zero, i.e. an excitation wave goes along the x- or y-direction. For the proposed design, BIC occurs when the $k_y$ component of wave vector is zero. Hence, in this case, the spectrum of the structure consists of pure TE and TM modes, see Fig. 1(b).

| (period,width) nm | $f$, THz (nm) | polarization | $\alpha_{\text{air}}$ (SiO$_2$) (deg) |
|------------------|-------------|-------------|------------------|
| (500,200)        | 241.2 (1243) | TM          | 65 (39)          |
| (600,270)        | 204.6 (1462) | TM          | 62 (38)          |
| (600,300)        | 197.2 (1520) | TM          | 74 (42)          |
| (600,240)        | 213.9 (1402) | TM          | 52 (33)          |
| (700,315)        | 186.6 (1607) | TM          | 49 (32)          |
| (700,280)        | 193.8 (1546) | TM          | 43 (28)          |
| (750,300)        | 185 (1621)   | TM          | 40 (27)          |
| (750,300)        | 186 (1612)   | TM          | 39 (26)          |
| (800,360)        | 172.6 (1734) | TM          | 41 (27)          |
| (800,360)        | 171.3 (1750) | TM          | 42 (28)          |
| (900,405)        | 161.9 (1851) | TM          | 33 (22)          |
| (900,405)        | 158.9 (1887) | TM          | 36 (24)          |

We consider the gratings fabricated from both silicon and silicon nitride. We numerically solved Maxwells equations by finite element method using COMSOL Multiphysics software.
One can see from Fig. 2 and Tab. 1 that there are many designs of grating supporting TE and TM-like BICs. We will choose one the most suitable for fabricating and experiment.

![Graphs showing BICs supported by silicon nitride grating](image)

**Figure 2.** Position of BICs supported by silicon nitride grating.

Also, we studied the influence of finite lateral size, i.e. finite number of periods, on frequency and Q-factor of both at-Γ and off-Γ BICs. In finite quasy-periodic array bloch wave vector ceases to vary continuously with in the first Brillouin zone but with step $\Delta k = \pi/aN$, where $N$ is a number of periods $a$ of the structure. Figure 3 shows dispersion curves and Q-factors. One can see that both at-Γ and off-Γ BICs keep the frequencies while the Q-factor drops significantly for off-Γ BIC. We suppose that the at-Γ BIC is less sensitive to finite lateral size due to protection by rotational symmetry. The finite structure has lost its rotational symmetry so the BIC transforms in resonant state with finite lifetime. But the more periods include the array the higher is it’s Q-factor.

To sum up, we have studied one-dimensional periodic structures. We confirm that the BIC transforms into resonant state with finite Q-factor due to finite lateral size of the structure. The obtained results provide useful guidelines for practical implementations of structures supporting optical bound states in the continuum and could find a number of applications in optical communications, on-chip photonics, laser physics and sensing.

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Figure 3. Calculated band structure and quality factor of silicon nitride grating supporting (a) TM-like BIC, (b,c) TE-like BIC.

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