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Theoretical study of light localization in photonic bandgaps of organic octagonal quasiperiodic photonic crystal slabs

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a r t i c l e i n f o

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A B S T R A C T

Based on the polystyrene material of low refractive index, light localization in photonic bandgaps of two kinds of 2D octagonal quasiperiodic photonic crystal slabs are investigated in theory, including the air-rod polystyrene slab and polystyrene-rod slab. The properties of bandgaps and localized modes in both two defect-free patterns are analyzed in detail. When a single-point defect is introduced into two quasiperiodic structures, the position of emerging defect modes and the red-shifting of resonant modes in wavelength are observed quite differently when the defect microcavity is increased in size. This difference is caused by the competition of two physical mechanisms, which are the effect of defect energy levels caused by defects introduced into photonic crystals and the resonance of modes in the defect cavity. These results will provide theoretical support for experimental fabrication of organic lightemitting quasiperiodic photonic crystal devices.

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1. Introduction

Following the pioneer works of John and Yablonovitch on periodic photonic crystals (PCs), quasi-periodic photonic crystals (QPCs) which consist of two or more materials arranged in quasiperiodic patterns have received much attention because of their remarkable properties. The structures of QPCs are not periodic but have long-range orientational order, so that it gives rise to a more isotropic Brillouin zone with smaller modulations that depress the gap [\[1\].](#page--1-0) Due to the greater rotational symmetry in QPCs, photonic bandgaps (PBGs) are independent of the incident light direction, which have potential applications in photonics $[2-5]$. Since the quasi-periodic arrangement has many in-equivalent local environments, the properties of defects are more complex and interesting than those created in conventional periodic PCs and may offer more flexibility in tuning the defect state properties $[6-8]$. For example, the light localization modes may occur in defect-free QPCs, which is useful for designing novel PC fibers and microcavities [\[9–11\].](#page--1-0) Besides, the dielectric constant necessary for the complete PBGs in QPCs is small. In the case of octagonal quasi-periodic lattice of dielectric rods in air, the first PBG for the TM polarization stays open down to the dielectric constant as small as ε = 1.6 (n = 1.26) [\[12\],](#page--1-0) while the threshold of the dielectric constant in dodecagonal QPCs is down to ε = 1.35 [\[13\].](#page--1-0) This property makes it possible that

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[http://dx.doi.org/10.1016/j.ijleo.2014.02.041](dx.doi.org/10.1016/j.ijleo.2014.02.041) 0030-4026/© 2014 Elsevier GmbH. All rights reserved. many PBG-based photonic devices can be fabricated from resourceful $SiO₂$ (n = 1.45) or organic polymer materials.

As we know, most of the PCs are made from III–V semiconductors. In contrast to inorganic optoelectronic materials, organic polymer materials, especially conjugated polymers, have advantages over the light-emitting property in the visible spectrum, the ease of fabrication and high optical nonlinearity. They have, therefore, become promising candidates as PC nano-lasers or light-emitting diodes $[14]$. Although the dielectric constant of organic materials is small, the combination of the light-emitting polymer and quasi-periodic structures with higher-level symmetry would provide better active layers, and more efficient, uniform in-plane confinement in all directions. Hence, it is beneficial for optoelectronic devices to achieve ultralow lasing threshold and high slope efficiency.

In this paper, we investigate the physical properties of PBGs and localized modes in 2D 8-fold symmetry QPC slabs at low-index contrast. By introducing a single-point microcavity into QPCs, we observe the dependence of localized resonant modes on the distribution of air-rods around a microcavity in polystyrene (PS) slab is quite different from that in PS-rods slab. The physical mechanism behind the difference and the fundamental parameters governing PBGs and resonant modes are discussed in detail.

2. Simulation and results

We design two kinds of 2D 8-fold symmetry organic QPC patterns, which are the air-rod PS slab and PS-rod slab, respectively.

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Fig. 1. Schematic patterns of 2D octagonal QPC slabs with air-rods in PS material (a) and PS-rods in air (b). The transmission spectra of Gaussian light in the corresponding structures (on the right).

Based on finite-difference time-domain (FDTD) method, we simulate the transmission of quasi-TE-polarized Gaussian light in the defect-free air-rod PS slab and quasi-TM light in the defect-free PSrod slab (see Fig. 1). The physical parameters of octagonal QPCs used in calculation are set as follows: the dielectric constant of PS material ε = 2.53 (n = 1.59), the lattice constant a = 260 nm, the rod radius $r = 65$ nm and the slab thickness $h = 400$ nm. Fig. 1 shows that even though the refractive index of PS is low, the bandgap still occurs in two kinds of slabs in the visible spectrum. Due to the high rotational symmetry of QPCs, several localized modes within the gap are observed in both defect-free structures. The origin of these peaks in QPC is attributed to the competition between two spatial structural properties: self-similarity and non-periodicity. If the effect of disorder resulting from the non-periodicity is dominant, the electromagnetic waves with some frequencies can be localized. The detailed explanation has been referred to our previous work in reference [\[9\].](#page--1-0) For the air-rod pattern, the PBG as shown in Fig. 1a is ranged from 532 to 619 nm and three peaks within the gap lie at 547, 556 and 589 nm, respectively. This spectral region is exactly corresponding to the fluorescence of conjugated PS at room temperature, which makes it possible for the fabrication of PC lasers and light-emitting diodes based on polymer as active layers. Different from that in the air-rod QPC slab, the bandgap of the PS-rod pattern covers the bluish-green region (442–495 nm) and only one mode is at 480 nm inside (see Fig. 1b). For all of the modes are at the band edge, the light localization is not obvious in the electric-field distribution.

Furthermore, we introduce a defect into QPC structures by removing a central scatter to form a single-defect photonic microcavity. Fig. 2 shows the corresponding transmission spectra of the modified octagonal QPC slabs with the thickness of 400 nm. Without a central air-rod, the PBG and resonant modes are almost the same as those in defect-free structures, including the location, width and transmission (see Fig. 2). In comparison, for the PS-rod structure in Fig. 2b, the original peak at 480 nm and PBG also stay the same, while a new defect mode at 486 nm arises from the lowfrequency band edge. The difference in property of two patterns is caused by the different average refractive index, even though the symmetry is the same.

Based on the single-defect microcavity, we then further shift the nearest-neighbor eight scatters around the cavity outward by

Fig. 2. Transmission spectra of 2D single-defect microcavity polymer octagonal QPC slabs by removing a central rod. Inset: schematic geometry of defect air-rods in PS material (a) and PS rods in air (b).

0.2*a*. It is clear to see in [Fig.](#page--1-0) 3a that two resonant modes in the gap are obviously red-shifting from 547 and 556 to 554 and 562 nm, respectively. Notice that the mode at 562 nm is moving close to the gap center and the quality factor Q of a cavity is increased significantly. [Fig.](#page--1-0) 3a shows the field pattern of electromagnetic waves at 562 nm which is well confined in the cavity. The localized state at 562 nm satisfies the constructive interference condition at the cavity boundary, so that even under the low refractive index, it still leads to the formation of the standing wave with in-plane confinement in all directions. According to Figs. 2a and 3a, it is therefore determined that the influence of the air-rods around a microcavity on the light localization is more effective than that of a central air-rod. For the PS-rod structure, however, the movement of nearest eight dielectric rods outward in [Fig.](#page--1-0) 3b hardly affects the PBG and modes. Then, we further remove the nearest eight scatters to construct a larger microcavity. It shows in [Fig.](#page--1-0) 4a that three modes keep red-shifting to 567, 569 and 599 nm, and a new mode emerges at 546 nm from the high-frequency band edge. However, the redshifting of resonant modes are not obvious in the PS-rod slab (see [Fig.](#page--1-0) 4b).

According to the simulated results above, we conclude two differences in property for two QPC slabs. One is that with the increase in the defect size, the red-shifting of resonant peaks in wavelength for the air-rod PS slab is more distinct than that for the PS-rod slab. The other is that a new defect mode emerges from the highfrequency band edge for the air-rod structure, while for the PS-rod structure, a mode arises from the low-frequency edge. The physical mechanism behind the differences can be explained by the band theory of solid physics. As we know, photonic crystals to manipulate beams are in the same way as semiconductors to control

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