NUMERICAL SIMULATION OF PHOTONIC CRYSTAL L3 NANOCAVITY

NGO THI PHUONG*, NGUYEN AN HOA**

ABSTRACT

We present a numerical study of photonic crystal L3 nanocavity based on silicon. The optical properties of L3 nanocavity are systematically investigated by using a plane-wave expansion and FDTD simulations.

Keywords: photonic crystal, silicon, L3 nanocavity, finite-difference time-domain (FDTD), plane wave expansion (PWE).

TÓM TẮT

Mô phỏng tính chất quang học của tinh thể quang tử có sai hỏng L3

Chúng tôi trình bày một nghiên cứu tính toán của tinh thể quang tử sai có sai hỏng L3 trên nền silic. Tính chất quang học của sai hỏng L3 được khảo sát một cách hệ thống bằng cách sử dụng các phương pháp mở rộng sóng phẳng và sai phân hữu hạn miền thời gian.

Từ khóa: tinh thể quang tử, silic, sai hỏng L3, sai phân hữu hạn miền thời gian (FDTD), mở rộng sóng phẳng (PWE).

1. Introduction

Photonic crystal (PC) is a structure in which a periodic variation in refractive index occurs at the scale of the wavelength of light in one or more directions [11]. In the situation where the refractive index contrast of the PC is sufficiently large, a photonic band-gap (a range of frequencies in which the propagation of light is forbidden) can be formed. The defect in such photonic crystals leads to the symmetry breaking of the structure. It is also possible to strongly localize light within a small volume [6]. Such defects are called nanocavities and characterized by small mode volume (V) and high Q-factor (Q). Photonic crystals are promising candidates to develop photonic devices in the near infrared spectral range. During the past two decades, a significant effort has been devoted to the study of two-dimensional (2D) photonic crystal both theoretically and experimentally for a variety of semiconductor materials.

Since silicon is the dominating material in current integrated circuit technology, various silicon-based nanocavity have been proposed in recent years. 2D photonic crystals using silicon are promising candidates for the development of silicon-based

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photonic devices. Cavities in silicon operate at telecommunication wavelengths, i.e. around 1.55 μm. Among photonic crystal cavity designs, the L3 nanocavity has widely been studied. This nanocavity consists of three missing air holes along the ΓK direction at the center of the triangular lattice. The longitudinal cavities such as L3 represent a good solution for optimizing the ratio *Q/V*. Because it was the first type of PC nanocavity in which quality factors exceeding 10^4 were obtained experimentally, the L3 nanocavity has been the subject of intense research for applications in cavity quantum electrodynamics (QED) [12], low-threshold lasing and control of ultrafast laser pulses [10, 2]. It is found that the L3 cavity is capable of supporting a multitude of modes: one fundamental mode and four high-order modes. High-*Q* modes can be obtained for the L3-type fundamental mode by carefully tuning the geometrical parameters and displacement of the first hole adjacent to the cavity [1, 4]. The improvement of *Q*-factor is explained by reducing the radiation losses compared to those with undisplaced holes. The higher-order resonant modes were paid a little attention. However, higher-order modes are important for the efficient pumping of nanocavity lasers, and also useful for the observation of cavity QED effects from single quantum dot coupled with high-*Q* nanocavities. In addition, the mode of the L3 nanocavity is "gently" confined within the spacer leading to a strong confinement of light inside the cavity. Due to its spatial flexibility, the L3 nanocavity is considered to be prevailing and beneficial for controlling the optical properties in different applications. These features make L3 defect one of the most widely used nanocavities by both experimental and theoretical researches for various purposes.

In this paper, we present the numerical analysis of photonic crystal L3 nanocavity using the silicon as a major material. The use of silicon photonic crystal L3 nanocavity presents thus a very high potential applications associated with Si-based photonic devices, including quantum information processing, filters and nanoscale sensors.

The format of the paper is as follows: In Section 2, we briefly describe model systems and the techniques used for the calculations. In Section 3, the results of our calculations for model systems are presented, the identification of the optical properties of a photonic crystal L3 nanocavity is emphasized. Finally, in Section 4 we summarize our results and give some discussions for future directions.

2. Design and calculation

a. Model design

The 2D model system is considered in our study with the hope of eliciting all the essential optical properties. 2D model means the system in which there is no variation in the fields or dielectric constant in the *z*-direction, and thus waves propagate only in the *x-y* plane.

One class of modes can be classified as transverse electric (TE) in which the magnetic field points in the *z* direction while the electric field lies in the *x-y* plane. The

other class is transverse magnetic (TM), in which the electric field points in the *z* direction and the magnetic field lies in the *x*-*y* plane.

We first investigate the properties of a cavity in a 2D photonic crystal. The crystal consists of a perfect array of infinitely long air-rods (hole) located in a triangular lattice of length of *a*. The dielectric constant chosen is 8.41, corresponding to an effective index $n_{eff} = 2.9$ of silicon. The type of cavity investigated is a missing-hole defect in a triangular host lattice (see Fig. 1). Each air hole has a radius of 0.3*a*. By normalizing every parameter with respect to the lattice constant *a*, we can scale the nanocavity to any length scale simply by scaling *a*.

b. Methods of computation

We applied two complementary schemes to deal with different aspects of the model systems. A frequency-domain approach is used to find the eigenmodes of perfect photonic structure as well as structure with defect. A time-domain approach was then applied to study the transient properties and the quality factor Q of the localized defect modes.

The propagation of light is governed by Maxwell's equations. A common approach to solve Maxwell's equations in photonic crystals is to look only for time-harmonic solutions and to exploit symmetries, in particular translation invariance, to simplify the equations for spectral problems with Schrödinger-type operators.

PWEM represents the periodic fields using a Fourier expansion in term of harmonic functions defined by the reciprocal lattice vectors wherein the application of the Fourier expansion turns Maxwell's equations into an eigenvalue problem. However, PWEM fails to simulate infinitely periodic structures, which is constrained by multiple symmetries and assumed the structure to be lossless. In addition, it is not capable of calculating the transmission and/or reflection spectra. Thus it is an effective tool to quickly determine the band-gap structure for both types of polarization, i.e. TE and TM.

The FDTD method is widely used to calculate transmission and reflection spectra for a general computational electromagnetic problem. It is generally considered to be one of the most applicable methods for photonic crystals. In this case, a wave propagating through the PC structure is found by a direct discretization of Maxwell's equations in point form, in which the partial differential equations are discretized in both time and space on a staggered grid. The boundary conditions then can be applied. In case the input signal is defined as continuous wave or pulse, the excitation can be propagated through the structure by time stepping through the entire grid.

An important feature is the ratio of the emission amplitudes collected from the surface between the different optical modes of the defect cavity. We calculate the theoretical radiation spectrum by using 3D-FDTD model. Within this model, the dipole emitters with a broad spectral range are inserted in the middle of the silicon slab.

Another important physical parameter measuring the sharpness of a resonator response is the quality factor *Q*. Generally, the quality factor is defined as the ratio of the average energy stored in the cavity and the energy loss,

$Q = \omega_0.E/P$;

where *E* is the stored energy in the cavity, ω_0 is the resonant frequency and *P* is the dissipated power (power loss). By computing $\Delta\lambda_0$ from photoluminescence calculation, the value of *Q*-factor is estimated as the ratio of the wavelength (λ_0) to the linewidth of the resonance ($Q = \lambda_0/\Delta\lambda_0$).

3. Results and discussion

3.1. Band diagram of photonic crystal L3 nanocavity

The L3 nanocavity consisting three missing air holes has the design shown Figure 1. The calculations are performed using a plane wave method with an interhole spacing of *a* and a hole radius of *r = 0.3a*.

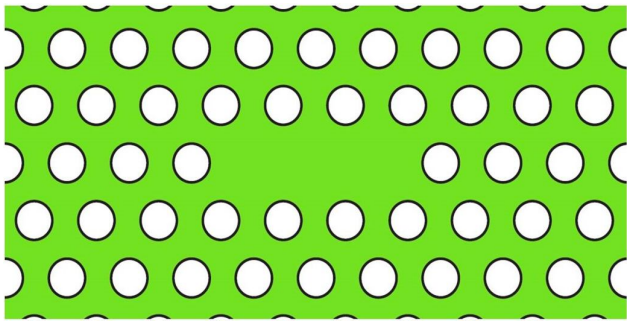

Figure 1. *A schematic representation of the 2D photonic crystal L3 nanocavity which is based on a three-missing-point defect in a triangular lattice. The lattice constant is a and the hole radius is r = 0.3a.*

Figure 2 shows the photonic band diagram for transverse-electric modes in a L3-defect triangular-lattice photonic crystal slab. The band gap is formed at normalized frequencies *u= 0.245 to 0.31* (i.e. 0.78 eV to 0.96 eV).

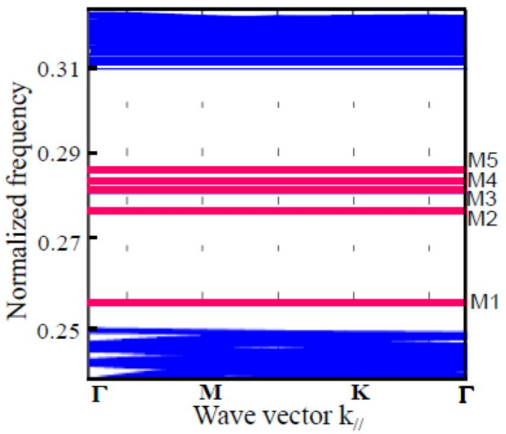

Figure 2. *Calculated dispersion diagram of a silicon photonic crystal L3 nanocavity. The white area corresponds to the photonic band gap. The defect modes of the L3 nanocavity which appear as horizontal pink solid lines in the gap, are numbered from M1 to M5.*

We note that the band gap spectral width can be adjusted by geometric parameters of photonic crystals. The presence of the cavity leads to the appearance of multiple resonances that modulate the photoluminescence spectra (transmission). These resonances correspond to the cavity modes (resonant modes) that are coupled with the leaky continuum modes. A defect state does indeed appear in the photonic band gap leading to a strongly localized state.

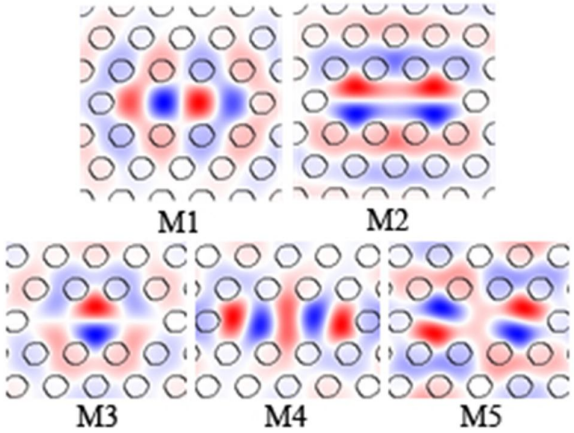

Figure 3. *The diagram shows the magnetic field distribution of resonant modes of L3 nanocavity, numbered from M1 to M5.*

Typical defect mode field with respect to patterns obtained from plan-wave expansion calculations are shown in Fig. 3. This result is in good agreement to other theoretical calculations. [4, 13]

Inside the photonic band gap of L3 cavity, five resonant modes were found in range of 0.797 – 0.889 eV. Of these, the fundamental mode M1 is the lowest-order mode which has the lowest energy and highest *Q*-factor. Four higher order modes (M2 – M5) are grouped together with the normalized frequencies of 0.274 – 0.287 higher than the fundamental mode.

The mode of interest in L3 nanocavity is fundamental mode (M1) due to high symmetric polarization in electromagnetic field distribution and stable energy level. The normalized frequency of this one is calculated at $u = a/\lambda = 0.245$. The resonant frequency of the cavity modes can be arbitrarily set by choice of the lattice parameter, *a*, and the air-hole radius, *r*.

3.2. Transmission spectrum of L3 nanocavity

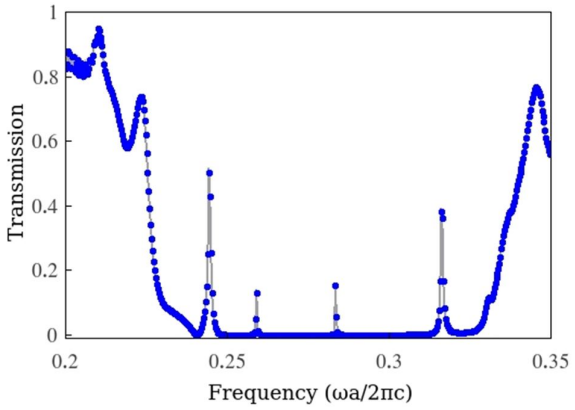

Figure 4. *Transmission spectrum of photonic crystal L3 nanocavity. A wide band gap can be seen in transmission spectrum. The gap extends from u = 0.245 to u = 0.32.*

Figure 4 shows the transmission spectrum for the silicon L3-cavity. This spectrum is obtained from 2D FDTD simulation. The photonic band gap, i.e. $u = 0.245 – 0.32$, is clearly visible in very low transmission range. We noted that the band-gap width in the transmission spectrum is in good agreement with the calculated value using a plane-wave expansion. This calculation reconfirms that the observed peak is due to the presence of a defect in a photonic crystal.

The spectrum consists of different sharp peaks corresponding to the resonant modes trapped in the defect. The position of the transmission peaks is found at $u = 0.245$, 0.28 and 0.32. They recover approximately the results of the corresponding resonant frequencies found in the band structure (as shown in Figure 2). The small discrepancy can be explained by the choice of computational coordinators between two methods.

It can be seen in the middle of the band gap that each mode of the defect is strongly localized at a resonant frequency. The resonant modes have an average

transmittance of 0.25, i.e. 25% of electromagnetic energy can be transmitted through the structure. As seen in the figure 4, the most significant resonant peak is located at the frequency of 0.257 coinciding with the frequency of the fundamental mode of L3 cavity. This mode presents high transmittance (T > 0.5).

The spectrum exhibits a number of interesting features: resonant modes, band-gap width, electromagnetic distribution, transmission coefficient. Such information make photonic crystal L3 nanocavity useful as a filter, mirrors, and for generating group delay. Thus, resonator structures in silicon photonic devices have been researched for their uses in optical filters, switches, and modulators

3.3. Photoluminescence spectrum of L3 nanocavity

In order to identify the radiation of resonant modes in the L3 nanocavity, 3D-FDTD are performed. The calculated photoluminescence spectrum for a L3 nanocavity is shown in the following figure.

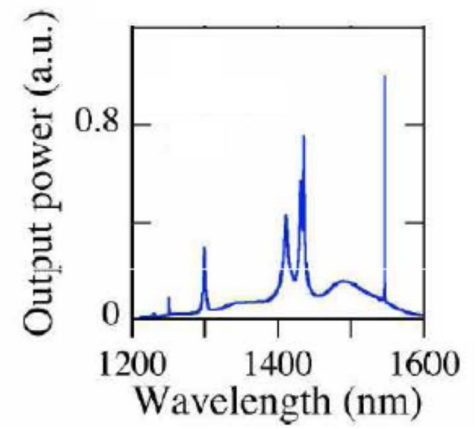

Figure 5. *Photoluminescence spectrum of photonic crystal L3 nanocavity*

Figure 5 shows the results of typical photoluminescence (PL) calculation on L3 cavity. The range of the PL spectrum is restricted to 1200 – 1600 nm in order to clarify the broad spectral luminescence of silicon. Within this range, we observed three main groups of modes for the L3 cavity: the first mode is observed at 1300 nm; the next mode is a group of three modes around 1400 nm and the last mode is at 1551 nm. These guided modes can enhance light emission over a large area because they are localized. The last peak presents the strongest resonant emission corresponding to the fundamental mode (λ = 1551 nm). We find that the PL peak intensity is enhanced by a factor of approximately 10 compared to the reference.

We note that our 3D-FDTD calculation enables to model a real structure in which the dipole emitters inserted in silicon slab play the role as the internal luminous sources. The design of the L3 nanocavity is based on air-bridge type photonic crystal slab which offers a strong light confinement.

The estimated full-width at half-maximum of the fundamental resonance is 0.3 nm, corresponding to a *Q* value of 5200, which coincides well with the experimental value [5]. The *Q*-factor value is one order of magnitude larger than those reported for others materials such as pure silicon on insulator [8], SiN on a buried oxide layer [3], and the germanium-on-Insulator type [9]. The lower quality factors may be limited by the weak confinement of light due to the small refractive contrast. In case of germanium nanocavity, the reason can be come from the strong absorption of pure germanium in the near infrared wavelength.

These results encouraged us to optimize the quality factor in the L3-type nanocavity by changing the position of the lateral edge air-holes around the defect. The quality factor can be also adjusted by displacing symmetrically the edge air holes. The emission can be tuned as a function of the lateral displacement the edge air hole [1, 5, 7]. It indicates that the resonant emission can be precisely controlled through the design of the cavity.

5. Conclusion

In summary, we have presented a brief description of techniques used for the photonic crystals L3 cavity on silicon. We have modeled the optical properties of the L3 cavity on silicon substrate using 2D PWE and FDTD calculation. The photonic bandgap of the triangular lattice for the 400 nm lattice and r/a = 0.3 cover the 0.245 – 0.33 spectral range in normalized frequency, i.e. corresponding to 0.78 – 1.02 eV or 1200 – 1600 nm, respectively. Using an effective index 2.9 for TE polarization at 1550 nm in the 2D plane-wave calculation, the fundamental mode of the L3 cavity is calculated at $u = 0.257$. FTDT simulation allows us to quantify the *Q*-factor and the photoluminescence and transmission spectra. The FDTD calculation predicts one at 0.257, i.e. 1551 nm instead of 1600 nm. The small discrepancy (3%) between two calculating values is attributed to the using the same effective index for all structure in PWE and a deviation from the nominal parameters. The present results support effort toward investigation of the optical properties for different types of photonic crystal nanocavity. These properties are essential for further discussion of potential applications to low-threshold nanocavity lasers and miniaturized photonic integrates circuits.

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