Fast algorithm for obtaining theoretical quality factor of two-dimensional photonic crystal cavity using mode profile

Akihiro Fushimi (M1)

We need to use the three-dimensional finite-difference time-domain method to obtain the $Q$ of a photonic crystal nanocavity. However, we need to calculate the total energy at every step to obtain an accurate $Q$, and this requires a large calculation cost. Here we study a method that can acquire the $Q$ of a two-dimensional photonic crystal nanocavity from a two-dimensional mode profile at the center of a photonic crystal slab without the need for a costly three-dimensional energy calculation. As a result, we can greatly shorten the calculation time.

Key words: Photonic crystal; FDTD; Algorithm.

1. Introduction

Today, we are becoming aware of the limitations of electronic devices. In contrast, photonic technology is attracting attention as a possible way of breaking through these limitations. Photonic crystal (PhC) nanocavities [1,2] are made by using semiconductor processes, and can be mounted on a Si slab because of their μm order size. So, the PhC nanocavity is regarded as a potential device for trapping and controlling light.

When we design a PhC nanocavity, we usually use three-dimensional finite-difference time-domain (3DFDTD) simulations. For this analysis, we obtain important cavity parameters including its resonant wavelength, and quality factor ($Q$). However, 3DFDTD consumes a lot of computational resources. Fortunately, we can parallelize the FDTD code, and so we can accelerate the calculation by using a parallel computer and graphics processing unit (GPU), which has many cores. In particular, GPU performance is improving greatly and the GPU price is low. To obtain the $Q$ factor of a cavity accurately, we need to calculate the total energy in the calculation area every calculation step. This calculation is difficult for a GPU to accomplish because it is poor at sequential computation, and so the required FDTD time becomes very long.

We propose a new method that obtains a $Q$ factor by using a 2D mode profile in the center of a PhC slab rather than a 3D energy calculation. Furthermore, our method can employ the mode profile as soon as the light sources finish their excitation, and we obtain the $Q$ factor even if the calculation area is small. Therefore, this method greatly reduces the calculation time.

2. Algorithm

The radiation losses of 2DPhC microcavities are the primary factor limiting the $Q$ factor. We obtain the in-plane momentum components $|k_\parallel|$ by using the spatial Fourier transformation of the mode profile in a cavity. The momentum components $k$ in a slab whose refractive index is $n$ is given as

$$k^2 = k_\parallel^2 + k_\perp^2 = \left( \frac{n\omega_0}{c} \right)^2$$

(1)

where $k_\parallel$ represents the vertical momentum components, $\omega_0$ is the angular frequency of light, and $c$ is the speed of light. The angle incident to the face of slab $\varphi_1$ is given as

$$\varphi_1 = \tan^{-1}\left( \frac{k_\parallel}{k_\perp} \right)$$

(2)

When $|k_\parallel|$ lies within the range

$$k_\parallel < \frac{\omega_0}{c} = k_0$$

(3)

the wave escapes to the air cladding because the light cannot satisfy the total reflection condition. This region is referred to as the light cone (LC) [3]. We improved the $Q$ factor by following the design principle that we need to reduce the number of the components in the LC [4,5]. However, there has been no evaluation study of the relation between LC components and $Q$ factor.

Our method estimates the loss rate by weighting each radiation mode component according to transmittance and the number of transmittances per second. First, the angle of refraction $\varphi_2$ is given as

$$\varphi_2 = \sin^{-1}(n \sin \varphi_1)$$

(4)

provided that we establish a vacuum around the slab. A PhC microcavity is usually coupled with a TE-like mode, so the amplitude transmittance $t_s$ is given as

$$t_s = \frac{2n \cos \varphi_1}{n \cos \varphi_1 + \cos \varphi_2}$$

(5)

Energy transmittance $T_s$ is given as

$$T_s = \frac{\cos \varphi_2}{n \cos \varphi_1} |t_s|^2$$

(6)

When thickness of the slab is $d$, the number of reflections per unit time $N$ is given as

$$N = \frac{c}{nd} \cos \varphi_1$$

(7)
The energy in the cavity $U$ is equal to the sum of each energy of TE mode’s $E_x$, $E_z$, and $H_y$.

$$U = U_{E_x} + U_{E_z} + U_{H_y} \quad (8)$$

The Q factor is defined as

$$Q = \frac{\omega_0 U}{|dU|/dt} \quad (9)$$

Our method uses a 2D mode profile when the energy is concentrated only in electric fields $E_x$ and $E_z$.

$$U_{E_x} + U_{E_z} = U, \quad U_{H_y} = 0 \quad (10)$$

We can get loss rate $L_{E_x}$ and $L_{E_z}$ by weighting of each of LC components according to transmittance and the number of transmittance per second. From Eqs. (8)–(10), $Q$-factor is given as

$$Q = \frac{U_{E_x} + U_{E_z}}{U_{E_x}L_{E_x} + U_{E_z}L_{E_z}} \quad (11)$$

From Eqs. (6) and (7), the loss rate is given as

$$L = \int_{LC} |E(k)|^2 \cdot T_s \cdot N \, dk \quad (12)$$

We use the effective refractive index $n_{eff}$ of each element as refractive index $n$ in the slab. $n_{eff}$ is given as

$$n_{eff} = \frac{\int_{all} k \cdot |E(k)|^2 \, dk}{k_0 \cdot \int_{all} |E(k)|^2 \, dk} \quad (13)$$

We approximate $U_{E_x}$ and $U_{E_z}$ with the following equation.

$$U_E = \int_{all} |E(k)|^2 \, dk \quad (14)$$

Equation (14) does not take account of the refractive index in real space because this equation means the summation in momentum space. However, we consider this problem by using the effective refractive index.

3. Results

First, we apply our method to an L3 resonator [4]. The design is shown in Fig. 1. The lattice constant $a$ is 420 nm, the air holes radius $r$ is 115.5 nm, and the slab thickness $d$ is 210 nm. The air holes in the side of resonator are shifted 32 nm from their original position, and their radius is 63 nm. The $xy$ plane, which passes through the center of the resonator, is a symmetry plane. The resonance wavelength is 1572 nm. The FWHM of the light source is about 3 nm. The spatial and momentum mode profiles are shown in Fig. 2. Fig. 3 shows the $Q$ factor obtained by the conventional method. Namely, it is calculated by decreasing the energy in the calculation area and applying our method. We apply our method when the light has just stopped, after 250 fs, and after 1 ps. The number of layers means the number of the rows between the resonator and the boundary of the calculation area.

When there are very few layers, the previous method normally estimates a lower $Q$ factor because the horizontal leak increases, and the energy moves outside the calculation area, so the loss rate is larger. On the other hand, our method makes it possible to obtain the “true $Q$ factor” that it is the $Q$ factor when the number of layers is infinity. Fig. 3 shows the number of layers versus the $Q$ factor of the L3 resonator.

So, we can shorten the calculation time by reducing the calculation area. Furthermore, we obtained a similar $Q$ factor when using the mode profile at different times (just as the light stopped, after 250 fs, and after 1 ps). This result shows we can obtain the $Q$ factor accurately even if we continue to calculate until the light stop as long as we set the light adequately. The conventional method requires us to continue calculating for a few ps after the light has stopped, but our method does not, so we can again shorten the calculation time.

Next, we apply our method to a width-modulated line defect nanocavity [6]. This design shows Fig. 4. Lattice constant $a$ is 420 nm, radii of air holes $r$ is 108 nm, and thickness of the slab $d$ is 205 nm. The shift of the air holes in the side of the resonator is 9-6-3 nm from their original position following. The plane of $xy$, which passes through the center of the resonator, is a symmetry plane. This resonance wavelength is 1568 nm. The light source’s FWHM is about 0.8 nm. The spatial and momentum mode profile shows Fig. 5. $Q$-factor getting by the usual method that calculates by decreasing the energy in the
calculation area and our method show Fig. 6.

Figure 6 shows \(Q\)-factor getting by two method is difficult when the number of the layer is 11, but Decay's value asymptote the value getting by our method, so when the number of the layer is larger, it is expected that the usual method's \(Q\)-factor is similar to our method's one.

![Fig. 5: The mode of width-modulated line defect nanocavity.](image)

![Fig. 6: The number of layers versus the \(Q\) factor of the L3 resonator.](image)

4. Calculation time

Finally, we show how we can reduce the calculation time. We perform a comparison using an L3 resonator and a width-modulated line defect nanocavity. We define the time required for the conventional method to be the calculation time until 1.25 ps after the light stops with energy calculated every step when there are 11 layers. The time required for our method is calculation time until the light stops without calculating energy when there are 5 layers. This result is shown in Fig. 7. Provided that we define this calculation time as (practical time)\(\times\)(the number of nodes), by using our method, we can shorten the calculation time by 1/4.2 with a L3 resonator, and surprisingly by 1/5.2 with a width-modulated line defect nanocavity.

![Fig. 7: Reduction of calculation time.](image)

5. Summary

We propose a new method that obtains the \(Q\) factor of a 2D PhC resonator by only a 2D mode profile at the center of a PhC slab. Our method can use the mode profile immediately after the excitation of the light source has finished, and we obtain the \(Q\) factor even if the calculation area is smaller. Therefore, this method greatly shortens the calculation time. This method allows the more efficient use of computer resources, and with an optimization algorithm, we can look for a higher \(Q\)-factor resonator.

References