Comparison of \(Q\)-Factors Between TE and TM Modes in 3-D Microsquares by FDTD Simulation

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Abstract—Mode characteristics of three-dimensional (3-D) microsquare resonators are investigated by finite-difference time-domain (FDTD) simulation for the transverse electric (TE)-like and the transverse magnetic (TM)-like modes. For a pillar microsquare with a side length of 2 \(\mu\)m in air, we have \(Q\)-factors about \(5 \times 10^3\) for TM-like modes at the wavelength of 1550 nm, which are one order larger than those of TE-like modes, as vertical refractive index distribution is 3.17/3.4/3.17 and the corresponding center layer thickness is 0.2 \(\mu\)m. The mode field patterns show that TM-like modes have much weaker vertical radiation coupling loss than TE-like modes. TM-like modes can have high \(Q\)-factors in a microsquare with weak vertical field confinement.

Index Terms—Finite-difference time-domain (FDTD) methods, microcavities, microsquare resonators, \(Q\)-factors.

I. INTRODUCTION

SQUARE optical microcavities have received a great deal of attention due to their potential applications for ultralow threshold and single-mode microlasers and high-finesse add–drop filters [1]–[8]. Multimode resonances were observed in square-shaped optical microcavities [1], single spatial-mode selection was realized in a layered square microcavity laser [2], and channel add–drop filters based on whispering-gallery (WG)-like modes in microsquare resonators were discussed [3], [4]. Mode characteristics for two-dimensional (2-D) microsquare resonators were theoretically analyzed and numerically simulated [5]–[7]. Furthermore, the mode characteristics in three-dimensional (3-D) microsquare resonators with strong vertical confinement were investigated numerically [8] and experimentally [9].

For a square resonator with the center in the origin point of Cartesian coordinates as shown in Fig. 1, we can assign modes as the transverse electric (TE)-like and the transverse magnetic (TM)-like modes based on their main polarization, although there are no real TE and TM modes in 3-D resonators. TE-like modes have symmetric electric fields and TM-like modes have antisymmetric electric fields relative to the middle plane \(z = 0\). The TE-like modes are the dominant modes in the microsquare resonators with strong vertical (\(z\)-direction) confinement. However, the TM-like modes should be considered in the resonators with weak vertical confinement. Recently, we analyzed mode characteristics for a 3-D microcylinder with different refractive index contrast in vertical direction [10], and found that the \(Q\)-factors of TM WG modes are much larger than those of TE WG modes in the microcylinder with weak vertical confinement. Due to the azimuthally symmetry, 3-D problem of the microcylinder can be transformed into a 2-D one in cylindrical coordinates and be simulated by 2-D finite-difference time-domain (FDTD) technique. However, real 3-D FDTD simulation is required for 3-D microsquare resonators. Furthermore, the break of the symmetries in the square would lead to some changes in the mode characteristics. In this letter, the mode characteristics of a microsquare resonator with weak vertical confinement are investigated by 3-D FDTD simulation.

II. NUMERICAL SIMULATION

Assuming the center layer thickness \(d\) is thin enough to support only the fundamental mode in the vertical direction, we can omit the mode number in the vertical direction and mark the TE-like (TM-like) modes as \(TE{(p,q)}\) (\(TM{(p,q)}\)), respectively, where mode numbers \(p\) and \(q\) denote the numbers of wave nodes of the \(z\)-direction magnetic field \(H_z\) (electric field \(E_z\)) in the \(x\)- and \(y\)-directions [5], respectively. The dominating components of electric (magnetic) field for TE-like (TM-like) modes are in the \(x\)-\(y\) plane similar to the practical TE (TM) modes in a 2-D resonator. As \(p-q\) is times of 2 but not zero, the corresponding modes are WG-like modes with \(Q\)-factors much larger than those of the other modes, and have antisymmetric field distributions relative to the diagonal mirror planes of the square [5]. We will focus on the WG-like modes in the following numerical simulation.

The microsquare resonator surrounded laterally by air is considered with the vertical refractive index distribution of \(n_2 = 3.17/n_1 = 3.4/n_2 = 3.17, d = 0.2 \, \mu\)m, and \(a = 2 \, \mu\)m. The reduced calculation region of one eighth of the resonator is

Fig. 1. Schematic diagram of one eighth of a microsquare resonator with vertical refractive index distribution of \(n_2/n_1/n_2\), center layer thickness \(d\), and side length \(a\).
shown in Fig. 1 bounded by the symmetry planes $\Sigma_{x}, \Sigma_{y}$, and $\Sigma_{z}$ at $x = 0, y = 0$, and $z = 0$. The perfectly matched layer (PML) [11], [12] absorbing boundary is used to terminate the other regions for the FDTD simulation. Considering the accuracy and calculation time, the PML boundaries are put at 0.5 $\mu$m and 5 $\mu$m away from the microsquare’s lateral and upper boundaries, respectively. A uniform mesh with cell size of 20 nm and a time step $\Delta t = 3.85 \times 10^{-17}$ s are used in the FDTD simulation. An exciting source with a cosine impulse modulated by a Gaussian function

$$P(x_0, y_0, z_0, t) = \exp[-(t - t_0)^2/\tau_w^2] \cos(2\pi f t)$$

is added to $H_z(E_z)$ at several points $(x_0, y_0, z_0)$ inside the microsquare for the TE (TM)-like modes, where $t_0$ and $\tau_w$ are the times of the pulse center and the pulse half width, and $f$ is the center frequency of the pulse. The Paéz approximation with Baker’s algorithm [13] is used to transform the FDTD output from the time domain to the frequency domain and calculate the mode frequencies and quality factors. The convergence of the intensity spectrum is realized as it does not vary with the length of the FDTD output.

We place perfect magnetic and electric walls on $\Sigma_{x}$ plane to excite TE-like and TM-like modes, respectively. 40 000-step FDTD simulation is performed and the intensity spectra are obtained from the FDTD output of the last 10 000 steps with the impulse at $t_w = 400 \Delta t$, $t_0 = 1000 \Delta t$, and $f = 200$ THz. The intensity spectra obtained under symmetry (antisymmetry) conditions relative to $\Sigma_{x}$ and $\Sigma_{y}$ planes are plotted as solid (dashed) lines in Fig. 2(a) and (b). The mode frequencies and $Q$-factors obtained by 3-D FDTD simulation are presented in Table I and compared with the results of 2-D FDTD simulation under the effective index (EI) approximation [8]. The mode $Q$-factors of $\text{TE}^{(4,6)}$, $\text{TE}^{(5,7)}$, $\text{TM}^{(4,6)}$, and $\text{TM}^{(5,7)}$ WG-like modes obtained by 3-D FDTD are 480, 380, 4.13 $\times 10^3$, and 6.54 $\times 10^3$, respectively. The results show that $Q$-factors of TM-like modes are about one-order larger than those of TE-like modes. The corresponding mode $Q$-factors obtained by 2-D FDTD simulation are 3.08 $\times 10^3$, 1.58 $\times 10^3$, 6.03 $\times 10^3$, and 2.26 $\times 10^4$, respectively, which are higher than those obtained by 3-D FDTD simulation, because the vertical radiation loss is not included in the 2-D FDTD simulation. For the TE-like WG-like modes, the vertical radiation loss results in about one order decrease of the $Q$-factors. However, for the TM-like WG-like modes, the vertical radiation loss is small and the $Q$-factors are still in the order of $10^3$. Assuming $1/Q_{3D} = 1/Q_{2D} + 1/Q_{t}$, where $Q_{3D}$ and $Q_{2D}$ are $Q$-factors obtained by 3-D and 2-D FDTD simulations, and $Q_{t}$ is $Q$-factor determined by the vertical radiation loss, we can obtain $Q_{t}$ to be 569, 389, 1.31 $\times 10^4$, and 9.20 $\times 10^3$ for $\text{TE}^{(4,6)}$, $\text{TE}^{(5,7)}$, $\text{TM}^{(4,6)}$, and $\text{TM}^{(5,7)}$ modes, respectively. The results show that the vertical radiation loss is the dominant factor in determining $Q$-factors for WG-like modes in the microsquare resonators. In addition, the mode frequencies of $\text{TE}^{(4,6)}$, $\text{TM}^{(4,6)}$, and $\text{TM}^{(5,7)}$ modes obtained by 2-D FDTD simulation are 5% to 13% larger than the 3-D FDTD results.

In order to understand the vertical radiation loss, we use a long optical pulse with narrow bandwidth to excite only one resonant mode, and obtain the field distribution by the 3-D FDTD simulation. We choose impulse (1) with $t_w = 8000 \Delta t$, $t_0 = 160000 \Delta t$, and $f$ of the corresponding mode frequency in Table I to excite only one single mode, and record the field pattern at the time of $t = 50 000 \Delta t$. The mode field distribution in the center plane ($z = 0$) is very different from those in the other planes far from the center layer. The obtained field patterns of the magnetic field component $H_z$ of $\text{TE}^{(4,6)}$ at $z = 0$ and 4 $\mu$m planes are plotted in Fig. 3(a) and (b), respectively. To recognize the field patterns, we also present the field patterns of 2-D analytical solutions [5] for $\text{TE}^{(4,6)}$ and $\text{TE}^{(5,6)}$ modes in Fig. 3(c) and (d).

| Mode Frequencies and $Q$ Values Obtained by 3-D FDTD and 2-D FDTD Under EI Approximation |
|-----------------|-----------------|-----------------|-----------------|-----------------|
|                | $f$(THz)       | $Q$            | $f$(THz)       | $Q$            |
| 3D              | $Q$            | 3D              | $Q$            | 3D              |
| $\text{TE}^{(4,6)}$ | 196.06        | 480             | 198.11         | 3.08 $\times 10^3$ |
| $\text{TE}^{(5,7)}$ | 227.46        | 380             | 229.91         | 1.58 $\times 10^3$ |
| $\text{TM}^{(4,6)}$ | 180.96        | 4.13 $\times 10^3$ | 183.24         | 6.03 $\times 10^3$ |
| $\text{TM}^{(5,7)}$ | 212.68        | 6.54 $\times 10^3$ | 215.40         | 2.26 $\times 10^4$ |

Fig. 3. Field patterns of the magnetic field component $H_z$ of mode $\text{TE}^{(4,6)}$ at (a) $z = 0$ and (b) $z = 4$ $\mu$m planes obtained by 3-D FDTD simulation, and analytical mode field distributions of (c) $\text{TE}^{(4,6)}$ and (d) $\text{TE}^{(5,6)}$.
which are almost the same as the field patterns of Fig. 3(a) and (d), respectively. The results show that \(TE^{(4,6)}\) mode coupled to a propagating mode in the cladding layer with the \(H_z\) distribution as mode \(TE^{(2,6)}\). In fact, the vertical radiation is caused by the mode coupling between \(TE^{(4,6)}\) and multiple propagating modes in the cladding layer with the same symmetry as \(TE^{(3,6)}\). So the field patterns in the cladding layer vary with the \(z\)-values.

The oscillation of obtained field distributions in the cladding layer indicates a vertical radiation loss. Because the field distribution in the \(z\)-direction is strongly relative to \((x, y)\) values, the vertical radiation loss cannot be described by the field distribution in the \(z\)-direction simply. So we introduce an effective amplitude distribution in the \(z\)-direction to describe the vertical radiation loss. The effective amplitude is defined as the square root of the average energy density in a \(z\) plane. The normalized effective amplitude distributions in the \(z\)-direction are shown as the dashed lines in Fig. 4 for (a) \(TE^{(4,6)}\) and (b) \(TM^{(4,6)}\) modes, and corresponding analytical field distributions of TE and TM modes in the three-layer slab waveguide are plotted as the solid lines, respectively. For \(TE^{(4,6)}\) mode, the effective amplitude only agrees well with analytical results when \(z < 0.3 \mu m\), and keeps a constant value of 0.12 as \(z > 2.5 \mu m\), which corresponds to the coupling with the propagating modes. For \(TM^{(4,6)}\) mode, the effective amplitude agrees well with analytical results, except has a very weak constant value of 0.02 as \(z > 3 \mu m\), which is much less than that of mode \(TE^{(4,6)}\). So the vertical radiation loss of \(TM^{(4,6)}\) mode is about one order smaller than that of \(TE^{(4,6)}\) mode, and TM-like modes still have high \(Q\)-factors in the microsquare resonators with weak vertical confinement. Different from the microcylinder [10], TM-like modes in the microsquare still have a weak coupling with the propagating modes, because the mode coupling between modes with different mode numbers \((p, q)\) is not forbidden in the microsquare. It should be noted that different vertical radiation losses for TE and TM modes are difficult to be explained by light scattering at corners, because it is based on the mode coupling of whole field pattern. We found that practically rounded corners at certain size can result in the increase of mode \(Q\)-factors in a 2-D square [14]. In the 3-D case, the \(Q\)-factors are mostly limited by the vertical losses, so the corners have a small influence on the \(Q\)-factors.

III. CONCLUSION

We have investigated the mode characteristics for microsquare resonators with weak vertical confinement by 3-D FDTD simulation. We found that vertical radiation loss strongly influences the \(Q\)-factors of the modes in the microsquares. TM-like WG modes have much less vertical radiation loss and higher \(Q\)-factors than TE-like WG modes. So we can expect an ultralow threshold microsquare laser formed by semiconductor materials based on the TM-like modes.

REFERENCES