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# Analysis of high- $Q$ photonic crystal L3 nanocavities designed by visualization of the leaky components

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**Abstract:** We experimentally study photonic crystal L3 nanocavities whose design  $Q$  factors ( $Q_{\text{design}}$ ) have been improved with the visualization of leaky components design method. The experimental  $Q$  values ( $Q_{\text{exp}}$ ) are monotonically increased from 6,000 to 2,100,000 by iteratively modifying the positions of some of the air holes, as determined by the referred design method. We investigate the  $Q_{\text{exp}}$  tolerance to imperfections in the fabricated samples, which reveals that the cavities improved by the visualization method tend to lose some tolerance to structural differences between the fabricated samples and the design values.

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**OCIS codes:** (230.5298) Photonic crystals; (140.3948) Microcavity devices.

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## 1. Introduction

High- $Q$  nanocavities in two dimensional photonic crystal (PC) slabs—which possess both high quality ( $Q$ ) factors and small modal volumes [1–5]—have attracted much attention in various fields, such as wavelength-selective filters [6,7], biosensors [8,9], optical pulse manipulation devices [10–13], solid-state cavity quantum electrodynamics [14–16], and low-threshold lasers [17–19]. In these applications, the high  $Q$  factors of the cavities are directly connected with desirable properties such as high resolution, high sensitivity, low operating energy, long pulse-memory time, and enhancements in nonlinear optical phenomena. Therefore, it is important to increase the  $Q$  factors of these cavities.

The L3 nanocavity—consisting of three missing air holes—is a very commonly used design for PC cavities [20,21]. In particular, L3 nanocavities with shifted air holes near the cavity edges are widely used in various research areas, because they can easily attain  $Q$  values in excess of a few tens of thousands [2,22], which are sufficient for many applications. Furthermore, L3 cavities have good connectability with PC line-defect waveguides, circular emission patterns, and small footprints [20–22]. On the other hand, their  $Q$  factors cannot be increased to the neighborhood of  $1 \times 10^6$ , a limitation that has reduced the potential of these

cavities. Recently, several methods have been proposed to obtain L3 cavities with design  $Q$  factors ( $Q_{\text{design}}$ ) larger than several million, and experimental  $Q$  factors ( $Q_{\text{exp}}$ ) larger than  $1 \times 10^6$  have been reported [23–25]. The potential of L3 nanocavities has therefore been steadily increasing.

Very recently, we proposed a simple method of increasing the  $Q_{\text{design}}$  of PC cavities, to which we called visualization method [26]. It consists of the following four steps: 1) Calculate the electric-field distribution for a cavity mode, with the three-dimensional (3D) finite-difference time domain (FDTD) method; 2) Fourier transform the electric-field distribution, to determine the leaky components within the light cone, not complying with the total internal reflection condition; 3) visualize the leaky components by inverse Fourier transforming them, thus determining the particular air holes that must be shifted to increase  $Q_{\text{design}}$  in the most effective manner; and 4) modify the air-hole positions in the leaky area, so as to decrease the leaky components. It was shown that by repeating the optimization rounds from Step 1 to Step 4, the  $Q_{\text{design}}$  values for L3 cavities have been consistently increased to several million [26].

In this paper we report on the experimental evaluation of L3 nanocavities designed by the visualization method. We fabricated nine types of L3 nanocavities, using progressively higher numbers of optimization rounds. With eight optimization rounds, the  $Q_{\text{exp}}$  values were consistently increased from 6,000 to 2,100,000, whereas the values of  $Q_{\text{design}}$  increased from 6,000 to 4,200,000. We also studied the  $Q$  value dependence on the radius of the air holes; remarkable decreases in  $Q$  were obtained when the radius departed from its design value.

## 2. Sample structure and design $Q$ factors

Figure 1(a) illustrates the measured samples, which consist of a triangular lattice of circular air holes on a thin silicon slab. The lattice constant  $a$  is 410 nm, and the thickness  $t$  of the slab is 217 nm. We fabricated three series of samples with different air hole radii  $r$ : 105, 110, and 115 nm; these values were confirmed by scanning electron microscopy (SEM). The excitation waveguide used to inject light into the cavity is 8% wider than the L3 cavity. Its separation ( $Dis$ ) from the cavity is different for different samples, so that the magnitude of the evanescent mode coupling between the propagation mode and the nanocavity modes can be controlled.

Figure 1(b) shows the structure details of the fabricated L3 cavities. The red circles indicate the shifted holes after the (up to eight) optimization rounds using the visualization method, whereas the dotted circles indicate their positions before being shifted. The numbers in each circle indicate the optimization round that led to the shift of that particular air hole, and the arrows indicate the shift direction. The optimization procedure is detailed in Ref [26]. Table 1 summarizes the shift magnitudes, the calculated values of  $Q_{\text{design}}$ , and the corresponding resonant wavelengths ( $\lambda_0$ ). In this table, the 0-round column corresponds to the normal L3 cavity, without any air hole shifts. As shown, the value of  $Q_{\text{design}}$  calculated for cavities with  $r = 110$  nm and  $t = 220$  nm increases monotonically from 0.006 million to 4.2 million. Although the shift magnitudes are the same of those in a previous study [26], the  $Q_{\text{design}}$  values are slightly decreased, because of the differences in the calculation parameters. We fabricated all L3 cavities (from 0-round cavities to 8-round cavities) on the same chip, with the fabrication procedure described in previous papers [4,15,19]. For comparison, we also fabricated, on the same chip, a multi-heterostructure nanocavity with a  $Q_{\text{design}}$  value of approximately 50 million [5]. The nanocavity was formed by a line defect of 17 missing air holes where the lattice constant in the  $x$ -direction was increased every two periods by 3 nm. In addition, the 8 air holes close to the cavity were shifted according to the visualization method [5]. The heterostructure nanocavity utilizes the modegap effect to confine the electric field in the  $x$  direction and therefore, the  $Q_{\text{design}}$  greater than 10 million is obtained [3,5].

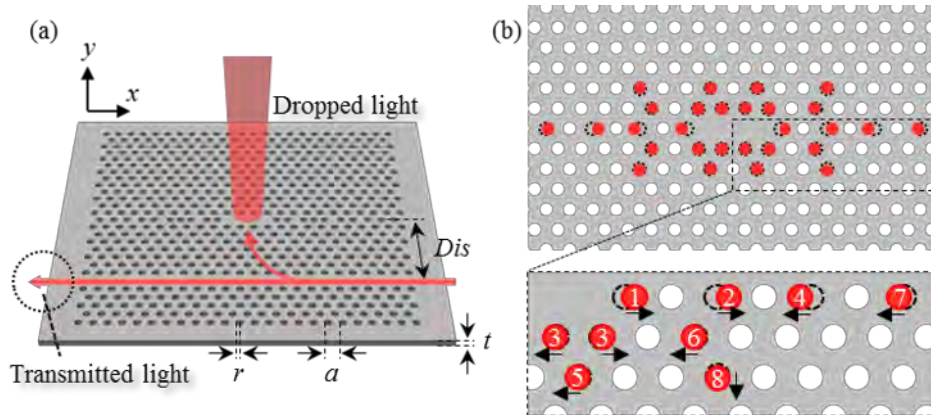


Fig. 1. (a) 3D schematic view of the samples where the L3 cavity and the excitation waveguide are formed. The light dropped from the cavity perpendicularly to the slab and the excitation waveguide transmitted light were both measured. (b) Details of the fabricated L3 cavities. The red circles indicate the shifted holes after the optimization rounds, whereas the dotted circles indicate their positions before the shift. The numbers in each circle indicate the optimization round that led to that particular shift.

**Table 1. Summary results for the air hole shifts,  $Q_{\text{design}}$  values, and calculated  $\lambda_0$ , for nine L3 cavities with  $r = 110$  nm. The 0-round column represents the normal L3 cavity, without air hole shifts.**

Round	0	1	2	3	4	5	6	7	8
Shift magnitude (a)	–	0.2	0.23	0.015 (outer) 0.005 (inner)	0.23	0.015	0.02	0.09	0.01
$Q_{\text{design}} (\times 10^6)$	0.006	0.13	0.25	0.48	0.96	1.6	3.1	3.6	4.2
$\lambda_0$ (nm)	1550.9	1564.3	1564.5	1565.8	1565.7	1565.2	1565.0	1565.0	1565.0

### 3. Experiments for cavities with a 110-nm radius

#### 3.1 Experimental results

To estimate the obtained values of  $Q_{\text{exp}}$ , we performed conventional spectral measurements on all cavities. The spectra of both the dropped and transmitted lights schematically shown in Fig. 1(a) were measured using a wavelength-tunable laser and a high-resolution wavelength meter. Details of the experiment were described in a previous paper [27]. Figures 2(a)-2(i) show the results obtained for the nine L3 cavities (from the 0-round to 8-round cavities respectively), with  $r = 110$  nm. The experiment was performed at room temperature, in standard air atmosphere. The black open circles in these figures represent the experimental data obtained for the dropped light, whereas the red curves show the transmitted spectra. The black solid curves are fitted curves (Lorentzian functions) used to evaluate  $\lambda_0$  and the full width at half maximum ( $\Delta\lambda_{\text{FWHM}}$ ). The shape of the drop spectrum in Fig. 2(a) is not symmetric because of the Fabry-Perot oscillation of the excitation waveguide. The blue curve represents the drop spectrum divided by the transmitted spectrum, which roughly reproduces an intrinsic resonant peak. The  $Q_{\text{exp}}$  values for the 0-round to 7-round cavities were estimated using the following relation [28]:

$$Q_{\text{exp}} = \frac{\lambda_0}{\Delta\lambda_{\text{FWHM}} \sqrt{T_0}}, \quad (1)$$



where  $T_0$  is the transmittance at the resonant peak.

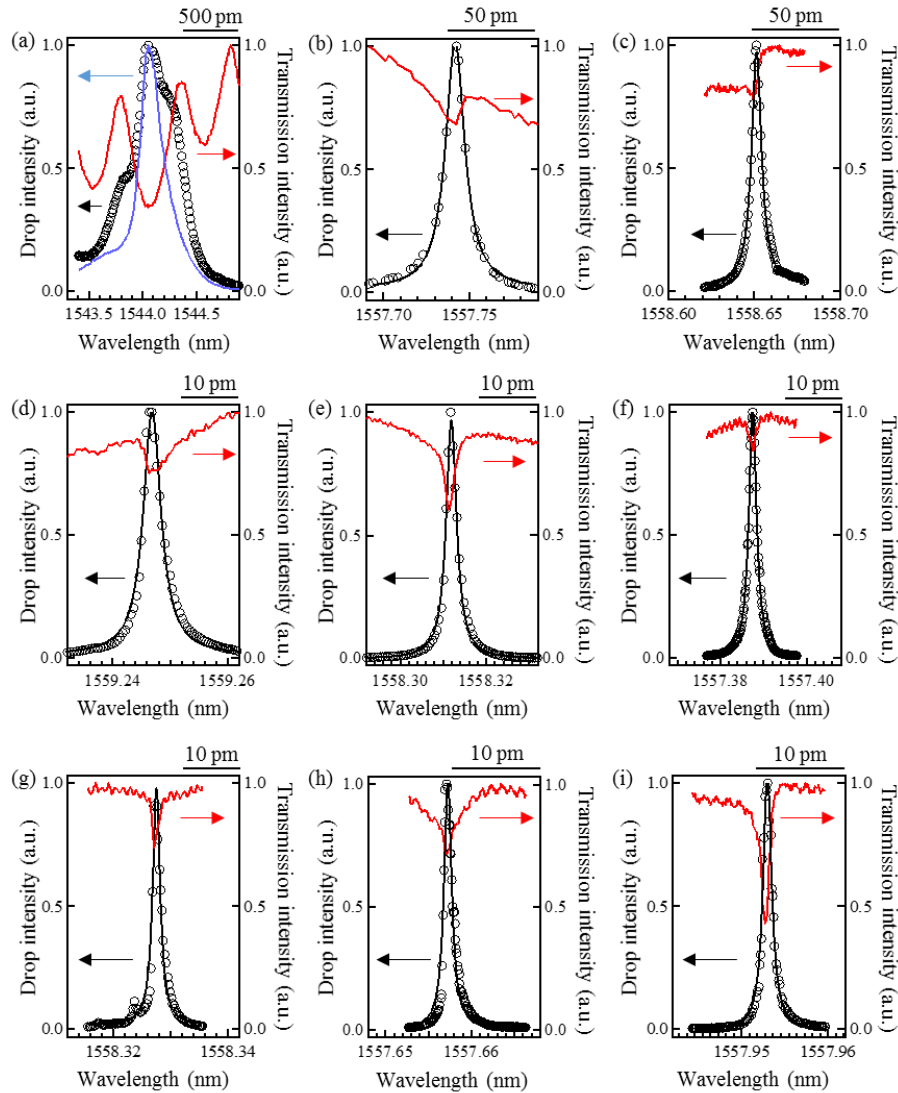


Fig. 2. (a)–(i) Dropped and transmitted spectra for the 0- to 8-round L3 nanocavities, respectively. Black circles represent the experimentally obtained results for the dropped light, whereas the red curves are the transmitted spectra. The black solid curves show the fitted Lorentzian functions. The blue curve in Fig. 2(a) is the drop spectrum divided by the transmitted spectrum.

In the spectral measurements, a temperature variation of the sample as small as 0.01 K may shift  $\lambda_0$  by as much as 0.8 pm. In addition, the Fano effect causes the asymmetric shapes of the drop peak and transmission dip [29]. These factors result in non-negligible error in the  $\Delta\lambda_{\text{FWHM}}$  determination. Therefore, to correctly evaluate the highest  $Q_{\text{exp}}$ , we used a time-domain approach to the measurements of the 8-round cavity. In the measurement, 5-ns-wide rectangular light pulses were applied to the excitation waveguide, and the time-domain evolution of the emissions from the cavity was measured using a photomultiplier tube and a time-correlated single-photon counting method. The experiment was also performed in standard air. Details of the measurement have been previously described in [5,30].

Figure 3 shows the time response of the 8-round L3 cavity, which indicates a photon lifetime  $\tau$  of 1.15 ns for the cavity.  $Q_{\text{exp}}$  was then estimated using the following relation:

$$Q_{\text{exp}} = \frac{\omega_0 \tau}{\sqrt{T_0}}, \quad (2)$$

where  $\omega_0$  is the angular frequency and  $T_0$  is the transmittance obtained from the spectral measurement.

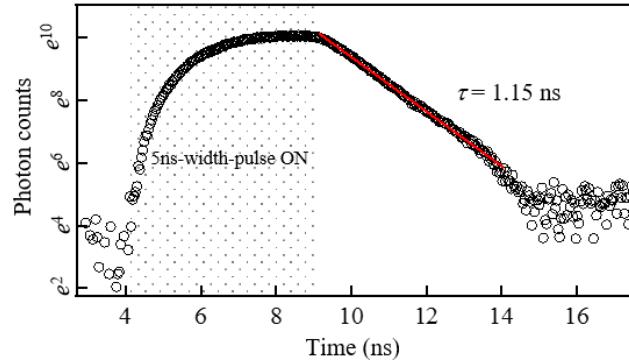


Fig. 3. Time-resolved signals for the nanocavity, with a 5-ns-wide pulsed light input. The shaded region corresponds to the pulsed input ON interval. The red fitted line indicates a 1.15 ns photon lifetime.

Table 2 summarizes the experimental results obtained with the nine L3 cavities. The  $\lambda_0$  shifts by 14 nm from round 0 to round 1, whereas it rarely changes from round 1 to round 8. This behavior agrees with the calculated results shown in Table 1. The value of  $Q_{\text{exp}}$  increases monotonically with the increase in the number of optimization rounds. It exceeds one million with six rounds, and reaches 2.1 million with eight rounds. This value is comparable to the highest  $Q_{\text{exp}}$  values ever reported for L3 cavities [25], and clearly demonstrates that the visualization method is useful for designing high- $Q$  PC cavities.

**Table 2. Summary measured results for the nine nanocavities: resonant wavelength ( $\lambda_0$ ), linewidth ( $\Delta\lambda_{\text{FWHM}}$ ), transmittance ( $T_0$ ), distance between the cavity and the excitation waveguide ( $Dis$ ), and experimental  $Q$  factor ( $Q_{\text{exp}}$ ). The  $Q_{\text{exp}}$  values for the 8-round and multi-hetero (MH) nanocavities are estimated from the photon lifetime obtained from time-domain measurements.**

Round	0	1	2	3	4	5	6	7	8	MH
$\lambda_0$ (nm)	1544.1	1557.7	1558.7	1559.3	1558.3	1557.4	1558.3	1557.7	1558.0	1576.5
$\Delta\lambda_{\text{FWHM}}$ (pm)	246	13.7	7.14	3.83	2.91	2.16	1.56	1.09	(1.15 ns)	(3.80 ns)
$T_0$	–	0.81	0.89	0.84	0.65	0.88	0.75	0.72	0.46	0.95
$Dis$ ( $\sqrt{3}a$ )	3.5	3.5	3.5	3.5	4.5	4.5	4.5	4.5	4.5	4
$Q_{\text{exp}}$ ( $\times 10^6$ )	0.006	0.13	0.23	0.44	0.66	0.77	1.2	1.7	2.1	4.7
$Q_{\text{imp}}$ ( $\times 10^6$ )	–	–	–	–	2.1	1.5	2.0	3.2	4.2	5.1

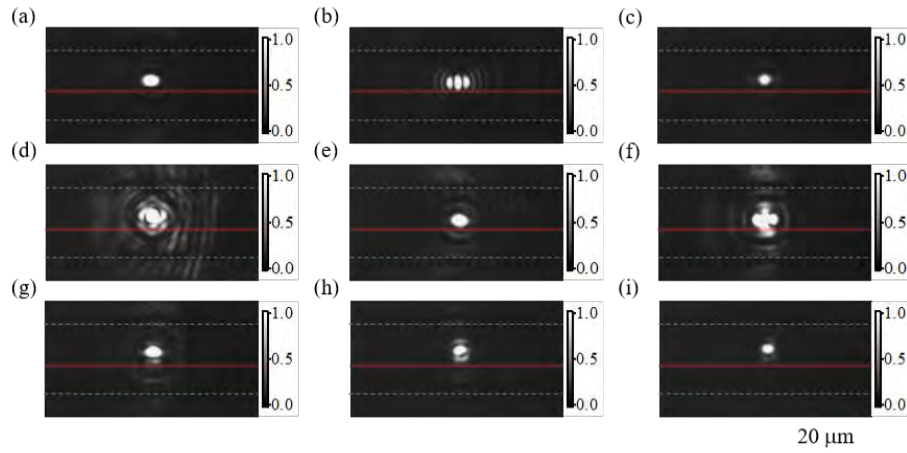


Fig. 4. (a)–(i) Near-infrared camera images of the 0-round to 8-round L3 cavities, respectively. The red lines represent the waveguides; the dashed lines indicate the PC pattern region interfaces.

Figures 4(a)–4(i) show near-infrared camera images for the 0- to 8-round cavities, respectively. A single-lobed spot was obtained for the normal (0-round) L3 cavity, and a sidelobed spot was obtained for the 0.2  $a$ -shifted 1-round L3 cavity, which is in good agreement with previously published studies [7,21]. Single-lobed spots were obtained for many cavities. Some distorted and split spots seem to be random effects resulting from the stochastic nature of the scattering caused by air hole fluctuations in radius and position, because they have not been reproduced in experiments with different samples.

### 3.2 Discussion for discrepancy between $Q_{exp}$ and $Q_{design}$

The discrepancy between  $Q_{exp}$  and  $Q_{design}$ —which is caused by the additional loss factors ( $Q_{imp}$ ) resulting from imperfections in the fabricated samples—should now be discussed [5,31–33]. The three  $Q$  factors are related by:

$$\frac{1}{Q_{exp}} = \frac{1}{Q_{design}} + \frac{1}{Q_{imp}}. \quad (3)$$

The reciprocal  $Q$  values are the optical losses. For cavities with  $1/Q_{design} \gg 1/Q_{imp}$ ,  $Q_{exp}$  should be approximately equal to  $Q_{design}$ . Such results are obtained for the 0- to 3-round cavities. The discrepancy becomes prominent for cavities with  $1/Q_{design} \cong 1/Q_{imp}$ , which corresponds to the 4- to 8-round cavities. The  $Q_{imp}$  values for these cavities derived from Eq. (3) are also presented in Table 2, and are distributed between 1.5 and 4.2 million.

We also measured the  $Q_{exp}$  values of 10 multi-heterostructure nanocavities fabricated on the same chip with  $a = 410$  nm and  $r = 110$  nm, using time-domain measurements. All the cavities possessed  $Q_{exp}$  values above 4.0 million; an average  $Q_{exp}$  value of 4.7 million was obtained, corresponding to a  $Q_{imp}$  value of 5.1 million, as results from Eq. (3). These results are also presented in Table 2. Since both types of nanocavities were fabricated on the same chip, the magnitudes of the imperfections must be the same. However, the values of  $Q_{imp}$  for the L3 cavities are lower than those for the heterostructure nanocavity and the variation of  $Q_{imp}$  for the L3 cavities seems to be large. These inconsistencies suggest that the L3 cavities designed with the visualization method lose tolerance to some structural imperfections.

Then, we performed 3D FDTD simulations to take the possibility of air-hole variations into account [32]. Normally distributed random nanometer-scale variations in position and radius were applied to all the air holes, with a standard deviation of  $\sigma_{hole} = 1$  nm. The average



value of  $1/Q_{\text{imp}}$  obtained for 30 different fluctuation patterns were almost identical for the 6-, 7-, and 8-round cavities:  $8.91 \times 10^{-7}$ ,  $8.90 \times 10^{-7}$ , and  $8.88 \times 10^{-7}$ , respectively. The standard deviation of  $1/Q_{\text{imp}}$  were also equal for the three cavities:  $4.26 \times 10^{-7}$ ,  $4.26 \times 10^{-7}$ , and  $4.19 \times 10^{-7}$ , respectively. On the other hand, the average value and the standard deviation for the multi-heterostructure nanocavity are  $6.91 \times 10^{-7}$  and  $3.03 \times 10^{-7}$ , respectively, which are somewhat smaller than the L3 cavities. These indicate that the L3 cavities have slightly lower tolerance to random structural disorders. However, it does not give a sufficient explanation for the inconsistencies of  $Q_{\text{imp}}$  values shown in Table 2. Another cause will be discussed below.

#### 4. Dependence of $Q$ on the air hole radius

##### 4.1 Experimental results

In this section, we will focus on the dependence of  $Q$  on the air hole radius. In fact, it is very difficult to fabricate PC samples with a given target radius with accuracies of (or above) 1 nm (e.g.,  $r = 110 \pm 1$  nm). This is because the final obtained radius is affected by several of the fabrication steps, such as electron beam lithography, development, and plasma etching. Furthermore, the radius of a fabricated PC sample is determined by SEM observations, whose accuracy is of only a few nm. Therefore, the dependence of  $Q$  on the radius is a core component of the tolerance to structural imperfections.

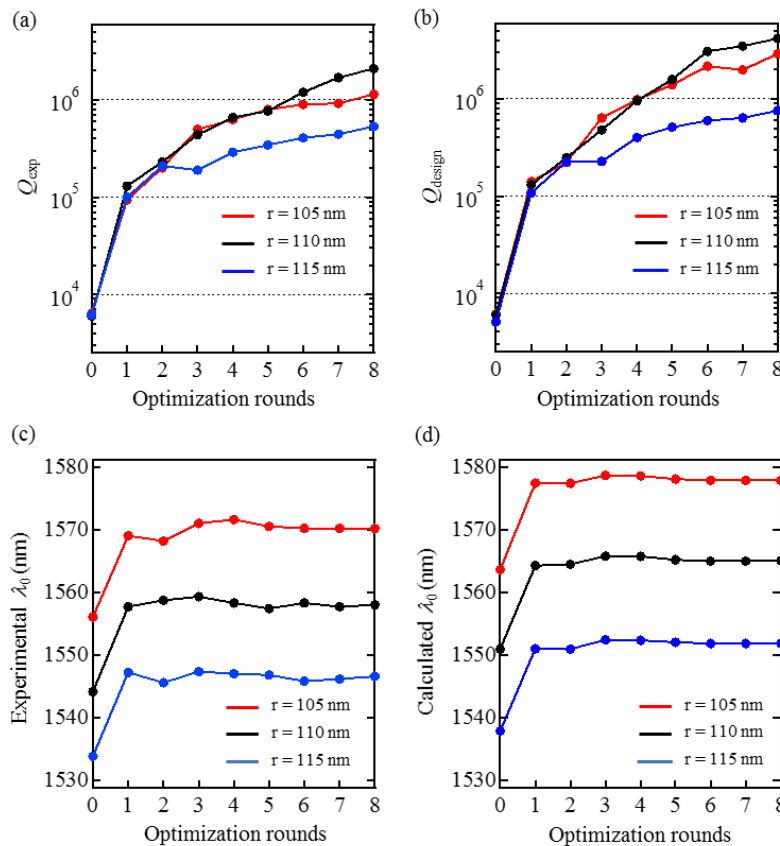


Fig. 5. (a) Experimental  $Q$  factors, and (b) calculated  $Q$  factors for three series of L3 cavities. (c) Experimentally obtained resonant wavelengths. (d) Calculated resonant wavelengths. The red dots, black dots, and blue dots represent cavities with  $r = 105$ , 110, and 115 nm, respectively.

We fabricated three different series of L3 cavities, with radii of 105, 110, and 115 nm. They have the same values for air hole shifts as those shown in Table 1. Figure 5(a) shows the corresponding values of  $Q_{\text{exp}}$ . As shown, up to round 2, the value of  $Q_{\text{exp}}$  is approximately the same in all three cases. In round 3, the cavity with  $r = 115$  nm exhibits a lower value than the other two, and the gap either increases or is maintained with the following rounds; the maximum value of  $Q_{\text{exp}}$  for  $r = 115$  nm is as small as 530,000, even in round 8. The cavity with  $r = 105$  nm has a smaller value in round 6 than the cavity with  $r = 110$  nm, and this gap increases in the following rounds; a maximum value of 1,140,000 is reached in round 8. Figure 5(b) presents the calculated values for  $Q_{\text{design}}$  using the 3D FDTD method; as can be seen, these results are consistent with the experimental results. Figures 5(c) and 5(d) present the experimentally obtained values of  $\lambda_0$  and their corresponding calculated values, respectively. As shown, they are in good agreement. The slight shifts in the absolute values can originate from small differences in radii and refractive index between experiments and calculations.

#### 4.2 Discussion for tolerance to structural design differences

Table 3 summarizes the results obtained for  $Q_{\text{exp}}$  and  $Q_{\text{design}}$ . It should be noted that the ratio of  $Q_{\text{design}}$  for  $r = 115$  nm and  $Q_{\text{design}}$  for  $r = 110$  nm is 0.91 in round 0, and decreases to 0.17 in round 8. Similarly, the ratio of  $Q_{\text{design}}$  for  $r = 105$  nm and  $Q_{\text{design}}$  for  $r = 110$  nm is 1.09 in round 0, decreasing to 0.51 in round 8. In general, the  $Q_{\text{design}}$  values for PC cavities increase with a decrease in the air hole radius. This is because the effective refractive index relative to the cavity mode field increases when the radius decreases, which enhances the light confinement by total internal reflection. The calculated results for a normal two-step heterostructure nanocavity with  $a_1 = 410$  nm,  $a_2 = 415$  nm, and  $a_3 = 420$  nm [3] are shown in Table 3. The  $Q_{\text{design}}$  values for the 110 and 115 nm radii are almost identical, with the  $Q_{\text{design}}$  for  $r = 105$  nm being greater than those two. On the other hand, the L3 cavities with  $r = 105$  nm have smaller values of  $Q_{\text{design}}$  when compared to the cavities with  $r = 110$  nm, for several numbers of rounds. It can therefore be concluded that the L3 cavities improved by the visualization method tend to decrease the tolerance to differences between the air hole radii of the fabricated samples and their design values. A similar tendency could be seen in the L3 cavities designed by the genetic optimization method [23]. Therefore, we suspect that this may be a universal characteristic of the improvement methods based on air hole shifts.

The value of  $Q_{\text{design}}$  is also influenced by differences in the slab thickness. The ratio of  $Q_{\text{design}}$  for  $t = 215$  nm and  $Q_{\text{design}}$  for  $t = 220$  nm is 0.98 in the 0-round L3 cavity with  $r = 110$  nm. The normal two-step heterostructure nanocavity also exhibits the same ratio. On the other hand, this ratio decreases to 0.89 in the 8-round L3 cavity. The shift and  $Q_{\text{design}}$  values shown in Table 1 were calculated using  $r = 110$  nm and  $t = 220$  nm, whereas the measured samples have  $t = 217$  nm. Furthermore, as discussed above, the radii have an uncertainty of a few nm, owing to SEM resolution limitations. These can be the main causes of the smaller  $Q_{\text{imp}}$  and the large variation observable in Table 2. The inconsistency between the refractive index used in the calculations and the one of the fabricated samples must also be considered in this discussion, because it will generate some errors in the optimal positions of the air holes.

The  $Q_{\text{exp}}$  does not seem to have reached saturation even with eight rounds as shown in Table 2. Additional optimizations via the visualization method would therefore further increase the highest  $Q_{\text{exp}}$ . However, we need to feedback the experimental results into the design calculation to adjust the differences between the calculations and the fabricated samples.

**Table 3. Summary results for  $Q_{\text{exp}}$  (upper row) and  $Q_{\text{design}}$  (lower row) for the nine L3 cavities and multi-hetero nanocavities (MH), with different air hole radii: 105, 110, and 115 nm.**

Round	0	1	2	3	4	5	6	7	8	MH
$Q (\times 10^6)$	0.006	0.09	0.20	0.50	0.63	0.80	0.90	0.92	1.1	–
$r = 105 \text{ nm}$	0.006	0.14	0.22	0.64	0.98	1.4	2.2	2.2	2.1	21.2
$Q (\times 10^6)$	0.006	0.13	0.23	0.44	0.66	0.77	1.2	1.7	2.1	–
$r = 110 \text{ nm}$	0.006	0.13	0.25	0.48	0.96	1.6	3.1	3.6	4.2	16.1
$Q (\times 10^6)$	0.006	0.10	0.21	0.19	0.29	0.34	0.41	0.45	0.53	–
$r = 115 \text{ nm}$	0.005	0.11	0.23	0.23	0.40	0.51	0.60	0.63	0.70	16.0

## 5. Conclusion

We demonstrated that the visualization method is useful for designing high- $Q$  PC cavities. Repeating the optimization round eight times, the  $Q_{\text{exp}}$  values of the L3 cavities were monotonically increased from 6,000 to 2,100,000. We also investigated the tolerance of the resulting  $Q$  factors to structural imperfections. It was shown that these L3 cavities tend to lose tolerance to structural differences in design, especially in what concerns the air hole radius. Our results show that the values of  $Q_{\text{exp}}$  about one million can be constantly obtained in the L3 cavities. Application area of L3 cavity will further extend.

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