Photonic crystal (PC) nanocavities with ultra-high quality ($Q$) factors and small modal volumes enable advanced photon manipulations, such as photon trapping. In order to improve the $Q$ factors of such nanocavities, we have recently proposed a cavity design method based on machine learning. Here, we experimentally compare nanocavities designed by using a deep neural network with those designed by the manual approach that enabled a record value. Thirty air-bridge-type two-dimensional PC nanocavities are fabricated on silicon-on-insulator substrates, and their photon lifetimes are measured. The realized median $Q$ factor increases by about one million by adopting the machine-learning-based design approach. © 2019 The Japan Society of Applied Physics

Statistical evaluation of $Q$ factors of fabricated photonic crystal nanocavities designed by using a deep neural network

Masahiro Nakadai$^{1*}$, Kengo Tanaka$^1$, Takashi Asano$^{1*}$, Yasushi Takahashi$^2$, and Susumu Noda$^{1,3}$

$^1$Department of Electronic Science and Engineering, Kyoto University, Kyoto 615-8510 Japan
$^2$Department of Physics and Electronics, Osaka Prefecture University, Sakai, Osaka 599-8570, Japan
$^3$Photronics and Electronics Science and Engineering Center, Kyoto University, Kyoto 615-8510 Japan

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Photonic crystal (PC) nanocavities with ultra-high quality ($Q$) factors and small modal volumes are anticipated for use in various scientific and engineering fields. The ratio $Q/V$ is a figure of merit for the strength of light–matter interactions and also for the photon lifetime in devices with small footprints, which are important parameters for various applications including nonlinear optics, quantum optics, and photonic buffer memories. As a high $Q$ is beneficial, there have been various efforts to increase the actual $Q$ factors of 2D-PC slab nanocavities.

In 2017, a record value of $1.1 \times 10^7$ for an experimental $Q$ factor ($Q_{\text{exp}}$) was reported for a silicon (Si)-based heterostructure nanocavity. This cavity was designed by using the leaky-mode visualization method, which is a manual design process, and positions of eight air holes were optimized with respect to the theoretical $Q$ factor. In 2018, a method based on machine learning for efficiently optimizing displacements of many air holes (fifty, in the present case) in nanocavities was proposed. By employing this method, which utilizes deep neural networks, a heterostructure cavity with an extremely high theoretical $Q$ factor of $1.6 \times 10^8$ has been designed. In this letter, we fabricate nanocavities with this new enhanced design and also nanocavities with the previous design in order to statistically compare their actual performances. Thirty cavities are fabricated for each design, and their $Q_{\text{exp}}$ are measured. It is shown that the distribution of $Q_{\text{exp}}$ significantly shifts to higher $Q$ factors by adopting the cavity design developed with the deep neural network: the ratio of cavities with $Q_{\text{exp}}$ larger than $9 \times 10^4$ (1 $\times 10^7$) increases from 12% (4%) to 28% (14%). Owing to the enhanced design, the median of $Q_{\text{exp}}$ is improved by about 1 $\times 10^5$, which significantly improves the fabrication yield.

The cavity designed by using the leaky-mode visualization method is shown in Fig. 1(a) (manual design; hereafter referred to as type M), and that designed by using the deep neural network is shown in Fig. 1(b) (hereafter referred to as type NN). The base PC comprises a triangular lattice of air holes formed in a 220 nm thick Si slab with refractive index $n = 3.46$. The radii of the air holes are 110 nm, and the base lattice constant $a_0$ is 410 nm. In each design, a cavity is formed by introducing a line defect with a certain length $L$ and a width $W1 = \sqrt{3} a_0$. The double heterostructure is obtained by symmetrically modulating the lattice constants $a$ in the $x$-direction as shown in Fig. 1; the spacings in the center and intermediate regions (each region spans two periods) are larger than $a_0$ (416 and 413 nm, respectively). Additional fine tuning of the air-hole positions is applied to increase the $Q$ factor: the design shown in Fig. 1(a) employs the displacements reported in Ref. 23. The design shown in Fig. 1(b) essentially employs the displacements reported in Ref. 26 [Fig. 8(d) in the reference] except for the discretization described below. The displacements of the air holes are shown by the black arrows in Fig. 1 and also in Tables I and II, where the amount of the displacements is discretized with a resolution of 0.125 nm, which is the resolution of the electron beam lithography (EBL) machine (JEOL JBX-6300) used for sample fabrication. The length $L$ of each cavity with the design shown in Fig. 1(a) is $17a$ in order to reproduce the structures in the previous reports. The other cavities with the design shown in Fig. 1(b) employ $L = 29a$, in order to avoid degradation of the theoretically predicted extremely high $Q$ factor due to the scattering at the ends of the cavity.

60 Cavities (30 for each type of cavity design) were prepared for this work. Each set of 30 cavities was fabricated on a single Si-on-insulator (SOI) substrate, whose top Si and buried oxide ($\text{SiO}_2$) layer thicknesses are 220 nm and 3000 nm, respectively. We note that the two types of samples were fabricated and measured at different times but the fabrication and data acquisition methods were the same. The layout of the samples is provided in Fig. 2(a); a long input waveguide with a width of $1.1 \times W1$ is shown near the bottom of the figure, and thirty cavities with the same design are located along this input waveguide with an interval of 20 μm. The distance between each cavity and the input waveguide is 6 rows in the $y$ direction. The block consisting...
Fig. 1. (Color online) (a) The manually designed double-heterostructure 2D-PC nanocavities used in this work, and (b) the design obtained using the deep neural network. Circles indicate the air holes with radii of 110 nm formed in the Si slab with a thickness of 220 nm. Displacements of air holes from the lattice positions are indicated by the black arrows (scale is shown on the right lower side). The distribution of the $y$ component of the electric field of the fundamental resonant mode is plotted with blue and red colors. The length of the cavity, $L$, is $17a$ for the design shown in (a) and $29a$ for the design in (b). In each design, an input waveguide with a width of $1.1$ is located at a distance of 6 rows from the cavity. The theoretical $Q$ factors including the load of the input waveguide for the structures in (a) and (b) are $2.8 \times 10^8$ and $1.8 \times 10^8$, respectively. The modal volume of each cavity is $1.5$ cubic wavelengths in the material.

Table I. Displacement data for Fig. 1(a).

| $X$ index | $Y$ index | $X$ shift (nm) | $Y$ shift (nm) |
|----------|----------|----------------|----------------|
| 0.5      | 1        | 0.000          | 0.375          |
| 2.0      | 2        | 0.875          | 0.000          |

Table II. Displacement data for Fig. 1(b).

| $X$ index | $Y$ index | $X$ shift (nm) | $Y$ shift (nm) |
|----------|----------|----------------|----------------|
| 0.5      | 1        | $-0.125$       | 0.500          |
| 1.5      | 1        | 0.250          | 0.000          |
| 2.5      | 1        | 0.250          | $-0.250$       |
| 3.5      | 1        | $-0.125$       | $-0.125$       |
| 4.5      | 1        | 0.000          | 0.375          |
| 5.5      | 1        | 0.250          | $-0.125$       |
| 0.0      | 2        | 0.000          | 0.125          |
| 1.0      | 2        | $-0.125$       | 0.000          |
| 2.0      | 2        | 0.875          | 0.125          |
| 3.0      | 2        | 0.125          | $-0.125$       |
| 4.0      | 2        | 0.250          | $-0.250$       |
| 5.0      | 2        | $-0.250$       | 0.250          |
| 6.0      | 2        | $-0.125$       | 0.250          |

of 10 cavities, as shown in Fig. 2(a), is repeated three times. The theoretical $Q$ factors including effects of coupling to the input waveguide are $Q_{\text{loaded}} = 2.8 \times 10^7$ and $1.8 \times 10^8$ for cavity type M in Fig. 1(a) and type NN in Fig. 1(b), respectively. The modal volume of each cavity is $1.5$ cubic wavelengths in the material ($\lambda/\sqrt{n}^3$). The values of $Q_{\text{loaded}}$ also include the effect of the finite $L$, and were calculated by the three-dimensional finite-difference time-domain (3D-FDTD) method. The details of the calculation are provided in Ref. 28. After the EBL process, the samples were subject to plasma etching. The buried oxide underneath the PC slab was removed by hydrofluoric acid (HF). This was followed by a surface treatment consisting of several repetitions of surface oxidation at elevated temperature and removal of the oxide by dilute HF (DHF). The details of the fabrication process are provided in Ref. 23. Figure 2(b) is a microscope image of the fabricated sample with cavities of type NN.

For statistical comparison of the two types of cavities, optical measurements were carried out in a chamber filled with dry inert gas, and the wavelengths $\lambda$ and photon lifetimes $\tau$ of the fundamental resonant modes of the cavities were determined. Each cavity’s $Q_{\text{exp}}$ is calculated using the relation $Q = 2\pi c \tau / \lambda$, where $c$ is the speed of light in vacuum. In order to avoid nonlinear effects, the pump power coupled into the waveguide facet was kept below $1 \mu$W. The details of the measurement method can be found in Ref. 23. We were able to detect the resonant modes of 25 cavities out of the 30 fabricated cavities of type M. With respect to the cavities of type NN, we were able to determine the $\lambda$ and $Q_{\text{exp}}$ of 29 cavities. The cavities that could not be characterized, most likely have too low $Q$ factors. Figures 3(a) and 3(b) plot the correlations between the obtained $\lambda$ and $Q_{\text{exp}}$ of the cavities employing the manual design (gray crosses) and the design developed with aid of the neural network (red dots), respectively. We confirmed that the $Q_{\text{exp}}$ of cavity type NN exhibited almost no change after the measurement (these samples were measured two weeks after the final DHF process, and the changes of $Q_{\text{exp}}$ over time were less than $2 \times 10^5$ within the following week). For a fair comparison, we should increase the values of cavities of type M, because there is a possibility that the measured values slightly underestimate the actual $Q_{\text{exp}}$ after sample aging. The data plotted by the crosses in Fig. 3(a) were measured one day after the final DHF process, but an increase of $Q_{\text{exp}}$ was observed for the best cavity: $Q_{\text{exp}}$ increased from $9.97 \times 10^6$ to $1.10 \times 10^7$ within three days. It is considered that the slowly proceeding evaporation of residual water on the cavity surface (during the storage in dry inert gas after the DHF process) reduces the absorption losses. Unfortunately, we were not able to re-evaluate all cavities. Instead, we employ
the following correction of the $Q_{\text{exp}}$ of the type M cavities:

$$Q'_{\text{exp}} = \left( \frac{1}{Q_{\text{exp}}} - \left( \frac{1}{9.97 \times 10^6} - \frac{1}{1.10 \times 10^7} \right) \right)^{-1}. \quad (1)$$

Here, $Q'_{\text{exp}}$ represents the corrected value. The blue dots in Fig. 3(a) correspond to the data pairs of $\lambda$ and $Q'_{\text{exp}}$, and we mainly use these corrected values in the following discussion. Figures 4(a) and 4(b) show the histograms of the cavity loss for the cavities of type M (data shown is the corrected $1/Q'_{\text{exp}}$) and for the cavities of type NN ($1/Q_{\text{exp}}$), respectively. Table III summarizes the relative occurrences of $Q_{\text{exp}}$ above a given threshold in the 25 cavities of type M and that of $Q_{\text{exp}}$ in the 29 cavities of type NN.

From the comparison of Figs. 3(a) and 3(b), we find that the average resonant wavelength of cavity type NN is only 8 nm larger than that of cavity type M. This indicates that the average air hole radii of both PC slabs are almost the same. From the observed difference of 8 nm, we can estimate a difference of less than 3 nm between the radii of the two types of samples using 3D-FDTD. Furthermore, the standard deviations of the resonant wavelengths of both cavity types are almost the same (0.44 nm for type M and 0.43 nm for type NN). This indicates that the magnitudes of the fluctuations in air-hole positions and radii are on the same order. In addition, the surface qualities (that is, those of top surface, walls of air holes, and especially the bottom surface) reached by the cleaning processes applied to the samples are considered to be on the same high level, because the highest $Q_{\text{exp}}$ observed in both samples is $1.1 \times 10^7$. Because the fabrication precisions and surface qualities of both samples are on the same order, the difference in the distributions of $Q_{\text{exp}}$ (or $1/Q_{\text{exp}}$) can be attributed to the difference in the cavity designs.

Comparison of the histograms shown in Figs. 4(a) and 4(b) reveals that the distribution drastically shifts to the lower cavity-loss side by adopting the new cavity design. Because the cavity loss (including effects of coupling to the waveguide) does not follow a normal distribution as shown in Fig. 4 (which is also confirmed theoretically, see Fig. 5), it is not appropriate to discuss the average values of $1/Q_{\text{exp}}$ or $Q_{\text{exp}}$ from the viewpoint of statistics. Instead, we directly compare the distribution of $Q_{\text{exp}}$ (corrected) of cavity type M with the distribution of $Q_{\text{exp}}$ of cavity type NN using the cumulative relative frequencies of $Q$ factors (Table III). The ratio of cavities with a $Q_{\text{exp}}$ larger than $1 \times 10^7 \times (9 \times 10^5)$ is only 4% (12%) for cavity type M while that of cavity type NN is 14% (28%). Furthermore, the percentage of cavities with $Q_{\text{exp}} > 8 \times 10^6$ (7.8 $\times 10^6$) is 28% (40%) for type M while that for type NN is 45% (62%). In addition, the median of $Q_{\text{exp}}$ increases almost by one million (from $6.9 \times 10^6$ to $7.8 \times 10^6$) when changing the cavity design from type M to type NN.

**Table III.** The center column provides those of $Q'_{\text{exp}}$ for the cavities of type M. The right column provides those of $Q_{\text{exp}}$ for the cavities type NN.

| $Q_{\text{exp}} \times 10^6$ | Type M | Type NN |
|-----------------------------|--------|--------|
| >10.0                       | 0.04   | 0.14   |
| >9.0                        | 0.12   | 0.28   |
| >8.0                        | 0.28   | 0.45   |
| >7.0                        | 0.40   | 0.62   |
| >6.0                        | 0.84   | 0.83   |
| >5.0                        | 0.96   | 0.97   |
| >4.0                        | 1.00   | 1.00   |
including effects of input waveguides and fluctuations of air-hole positions and radii. The histograms of the increase of the loss caused by the fluctuations, \( \Delta Q/Q = Q_{\text{loc}} - Q_{\text{ideal}} \), are shown with the thin lines.

This means that the yield of obtaining extremely high \( Q_{\text{exp}} \) (>7 \( \times \) 10^6) is largely improved by adopting the cavity design developed with the deep neural network. We consider that a more complex pattern of hole displacements is able to realize a mode distribution that more effectively reduces losses that can be derived from the cavity design.

To better understand the origin of the distributions observed in Fig. 4, we theoretically estimated the effects of fabrication inaccuracies by calculating the \( Q \) factors for cavity structures including fluctuations of air-hole positions and radii with a standard deviation 0.001 \( a \). For accurate comparison, we applied 1000 different fluctuation patterns (every pattern defines a unique set of relative offsets from the ideal structure parameters) to each cavity type. Figures 5(a) and 5(b) show the histograms of the theoretical cavity loss (1/\( Q \)) determined by 3D-FDTD for type M and type NN cavities, respectively. The bars represent the frequencies of occurrence of the derived cavity loss 1/\( Q_{\text{loc}} \), which include both the coupling to the input waveguides and the additional losses induced by fluctuations of air-hole positions and radii.

The lines in Fig. 5 show the distribution of 1/\( Q \) calculated by 1/\( Q_{\text{loc}} \) – 1/\( Q_{\text{waveguide}} \), where the \( Q \) factors of the ideal structures including coupling to the input waveguide (but without fluctuations) are \( Q_{\text{waveguide}} = Q_{\text{loaded}} = 2.8 \times 10^7 \) and 1.8 \( \times \) 10^8 for type M and type NN, respectively. It is interesting to note that the distributions of 1/\( Q \) for both cavity types are similar. Therefore, an improvement of the cavity design can lead to an actual improvement in \( Q \) factors of fabricated samples. Comparison between the experimental data in Fig. 4 and the 1/\( Q_{\text{loc}} \) of Fig. 5 reveals that the predicted ranges for the plateaus of the distributions (1.1–1.6 \( \times \) 10^{-7} for type M and 0.9–1.3 \( \times \) 10^{-7} for type NN) are in fair agreement with the experiment. Although we were not able to observe cavities with losses less than 0.9 \( \times \) 10^{-7} in the experiment, the fair agreement suggests that the significantly lower 1/\( Q_{\text{loaded}} \) of the type-NN design is also reflected in the 1/\( Q_{\text{exp}} \) of the fabricated cavities.

In conclusion, we experimentally investigated the \( Q \) factors of air-bridge-type Si-based 2D-PC nanocavities with a new design developed with a deep neural network. To investigate the advantages of this machine-learning-based design approach, we compared the results with those obtained from cavities that employ a design that has previously been developed with a manual approach. The fabrication yield of cavities with experimental \( Q \) factors larger than 1 \( \times \) 10^7 was improved by a factor of more than three (from 4% to 14%) by adopting the new design. This is mainly because a deep neural network is able to optimize more air-hole positions as compared to what can be optimized by a manual approach within feasible time. Owing to this design approach, the loss determined by the cavity design itself is significantly reduced and the median of the experimental \( Q \) factors was improved by about 1 million (from 6.9 \( \times \) 10^6 to 7.8 \( \times \) 10^6). We believe that optimization with aid of a deep neural network can also increase the experimental \( Q \) factors of other types of nanocavities, which will be useful in various scientific and engineering fields.

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27. Although Ref. 23 reports that the loaded \( Q \) factor of this cavity is forty million, the value that takes the presently used discretization of the air-hole shifts and finite length of the cavity into account, is 2.8 \( \times \) 10^7. Additionally, the modal volume of the presently used cavity is 1.5 \( \times \) 10^-4 m^3.
28. To perform the 3D-FDTD simulation, we used a calculation domain with dimensions of 4\( \times \) 4\( \times \) 17\( \sigma \) (\( x, y, \) and \( z \) directions, respectively), where \( \sigma \)
is the lattice constant. The cell size is about 0.1\(a\) in each direction and the time step \(\Delta t\) is 0.05\(a/c\) (\(c\) is the speed of light in vacuum). In addition, for the discretization of the distribution of the dielectric constant in the FDTD calculation, we employed a sub-cell size of about \(a/4000\) and the dielectric constants of each cell was determined by averaging over its sub cells. The \(Q\) factors are determined by calculating the ratio of energy in the cavity to leaked power. The outlined method is sufficient to calculate \(Q\) factors up to \(5 \times 10^8\).

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