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Design of a three-dimensional photonic crystal nanocavity based on a <110>-layered diamond structure

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Abstract

We design a novel three-dimensional (3D) photonic crystal (PC) nanocavity based on a <110>-layered diamond structure. The designed structure, comprised of self-sustainable layers, is suitable for fabrication by a layer stacking technique. Numerical simulations indicate that the quality factor of the designed nanocavity with 35 stacked layers can reach as high as 250,000. This value is 2.4 times higher than that of a conventional 3D PC nanocavity based on a woodpile structure with the same in-plane size and with the same number of stacked layers.

1. Introduction

Three-dimensional (3D) photonic crystals (PCs) composed of spatially periodic arrangements of refractive indices can exhibit complete photonic bandgaps (cPBGs), in which light propagation with any polarization is prohibited omnidirectionally. Artificially introduced defects in the perfect crystals create localized states of photons in the cPBG and work as optical waveguides or nanocavities. These could be key tools for realizing the ultimate control of photons on the wavelength scale. In particular, high-Q nanocavities in 3D PCs are anticipated as a platform for exploring light-mater interaction in a completely engineered electromagnetic environment, which can lead to various potential applications such as low threshold lasers [1] and quantum information processing devices [2,3].

The highest experimental Q-factor in a 3D PC nanocavity (~39,000) was achieved in a semiconductor-based woodpile 3D PC structure [4], which is the structure mainly investigated among various types of 3D PCs due to its structural simplicity and large cPBG. However, higher Q-factors are still desired for the aforementioned device applications. In addition to Q, the total size of the structure is another important issue to be considered. Nanocavities with higher Q in a limited size allow for dense integration for future applications. From a fabrication point of view, this is also an essential issue: The micro-manipulation technique[5] is a promising method for the fabrication of high-quality 3D PCs at present (indeed it was used for the demonstration in [4]), but cannot be used effectively to fabricate 3D PCs with a larger in-plane size.

In this study, therefore, a novel 3D PC structure based on a <110>-layered diamond structure [6, 7] is investigated to improve Q-factors in 3D PC nanocavities whilst maintaining a finite in-plane size. First, the cPBG of the <110>-layered diamond structure is maximized by optimizing the structural parameters using the plane wave expansion (PWE) method. Then, we introduce a square-shaped cavity in the structure and calculate the Q-factor using the finite-difference time-domain (FDTD) method. We find that a maximum Q of ~250,000 can be attained with this novel 3D PC nanocavity. This value is 2.4 times higher than that of a conventional 3D PC nanocavity with the same in-plane size and with the same number of stacked layers.

2. <110>-layered diamond and woodpile structure

The <110>-layered diamond structure is a simplified diamond structure sliced into four layers along the <110> direction [6, 7]. For comparison, the woodpile structure is another simplified diamond structure, though sliced into four layers along the <100> direction (for this reason it is sometimes called as <100>-layered diamond structure).

Figure 1(a) shows a schematic of the examined 3D PC nanocavity based on a <110>-layered diamond structure. In order to fabricate it using the micromanipulation technique, the structure is separated into plates with self-sustainable patterns, in contrast to ref [6]. The plate pattern is shown in Fig. 1 (b). The pattern consists of periodic rods which are connected to the frame of a plate and are separated by $a_{<110>}$. The pattern also has a triangular array of cylindrical holes penetrating in the stack direction. Thus, each rod is not straight as shown in Fig. 1(b). The patterns on two neighboring plates are shifted by $a_{<110>}/2$ in the z direction with respect to each other (see the bottom illustration in Fig. 1 (b)). Since the cPBG is maximized when the unit cell of

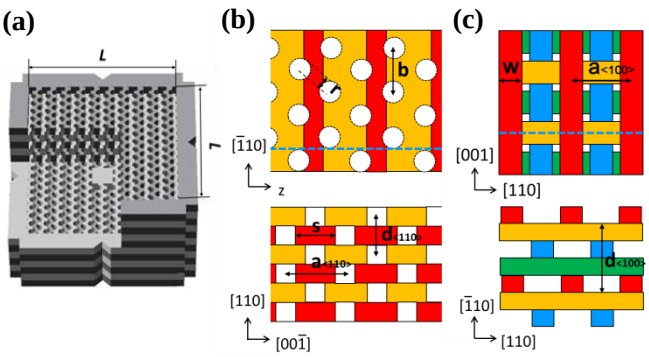

Fig. 1 (a) Bird's eye view schematic of the 3D PC nanocavity based on the <110>-layered diamond structure. The structure is partially cut for clarity. (b), (c) Schematics of the partial patterns from the top view point (top) and from the side view point (bottom) of the <110>-layered diamond (b) and of the woodpile structures (c).

the 3D PC is a face-centered cubic (FCC) lattice [6, 8], the structural parameters are set as $b = d = a_{<110>}/\sqrt{2}$. Here, b and d are the periods of the arranged cylindrical holes in the in-plane and the stacked directions, respectively. Other parameters, such as the radius of the holes (r) and the width of rods (s) are also defined in Fig. 1(b).

We also consider a 3D PC based on a conventional woodpile structure as shown in Fig.1 (c). Straight rods with a width of w are separated by $a_{<100>}$. The periods in the stack direction $d_{<100>}$ follows $d_{<100>} = \sqrt{2}\,a_{<100>}$, thus forming a FCC lattice. It is worth noting another important difference between the two structures, namely that the number of different types of plates making one period along the stacked direction is two for the <110>-layered diamond structure and four for the woodpile structure, as shown in different colors in Fig. 1 (b) and (c). This will be an advantage of the <110>-layered diamond structure from the fabrication point of view. In both structures, the in-plane size of the pattern is set to be finite as an $L \times L$ squared region shown in Fig. 1(a).

3. Results and discussions

First, we maximize the cPBG of both 3D PC structures without nanocavities by the PWE method. Figure 2(a) and (b) show the cPBG ($\Delta\omega/\omega$) as a function of the filling ratio $s/a_{<110>}$ for the <110>-layered diamond and $w/a_{<100>}$ for the woodpile structure, respectively. Here, $\Delta\omega$ and ω are the frequency width of the cPBG and the center frequency of the cPBG, respectively. We obtained a maximum cPBG of $\Delta\omega/\omega$ = 15.9% in the <110>-layered diamond structure. This is slightly smaller than that in the woodpile structure ($\Delta\omega/\omega$ = 18.9 %).

We next introduce a square-shaped cavity at the center of the middle layer of the optimized 3D PCs. We focus our attention on the first confined mode to appear as the defect size is increased from zero. Here, the in-plane size of both patterns is set as L = 3.63 μm, and the lattice constant of both structures is $a_{<110>} = \sqrt{2}a_{<100>}$ = 0.5 μm, ensuring that both structures mimic the same ideal diamond lattice with a lattice constant of 0.5 μm. The size of the cavities is optimized in each structure so as to tune the cavity mode wavelength close to the center of the cPBG, which maximize the Qs of each structure. The optimized cavity size is 0.009 um^3 for the <110>-layered diamond structure and 0.013 um^3 for the woodpile structure. The cavity wavelengths are around 945 nm for both structures.

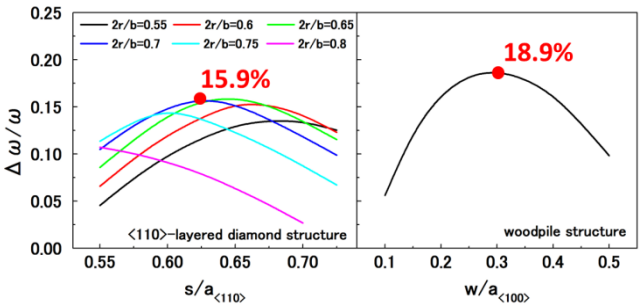

Fig. 2 Complete PBG as a function of filing ratio for the <110>-layered diamond (a) and for the woodpile structures (b).

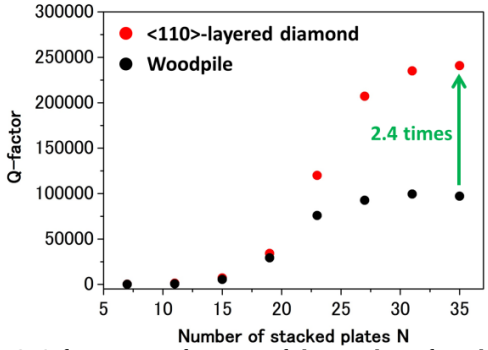

Fig. 3 Q-factors as a function of the number of stacked plates with the optimized cavities in <110>-layered diamond and woodpile structures.

Figure 3 shows the calculated Q-factors as a function of the number of stacked plates for both structures. The Qs of both structures initially increase with the number of layers due to the increasing number of periods in the stacking direction, before finally saturating due to the finite plate size. The saturated Q-factor of the 3D PC nanocavities based on the <110>-layered diamond structure reaches as high as 250,000, which is 2.4 times higher than that of the conventional woodpile structure.

Although the cPBG in the <110>-layered diamond structure is narrower than that in the woodpile structure, its Q-factor is higher. One of the possible reasons for this counterintuitive result is the difference in the number of unit cells of original diamond lattice in the plate. In the same $L \times L$ in-plane size, the <110>-layered diamond structure contains ~$\sqrt{2}$ times the number of the cells of the woodpile structure due to the difference of in-plane rod period.

3. Conclusions

In this study, we have investigated a 3D PC nanocavity based on the <110>-layered diamond structure tailored to be suitable for fabrication by a micro-manipulation technique. Compared with the conventional woodpile structure, the novel layer-by-layer structure potentially exhibits a 2.4 times increase in Q (up to ~250,000) with 35 stacked layers and the same in-plane size obtained by the numerical calculations.

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References

[1] G. Bjork and Y. Yamamoto, *IEEE J. Quantum Electron.* **27**, pp. 2386-2396 (1991).

[2] H. Mabuchi and A. C. Doherty, *Science* **298**, 1372 (2002).

[3] S. J. van Enk *et al*,. *Springer Science+Business Media, Inc*, **3**, pp. 75-90 (2004).

[4] A. Tandaechanurat, *et al*., *Nature photon*. **5**, 91 (2011).

[5] K. Aoki *et al*., *Nature Mater*. **2**, 117 (2003).

[6] S. Fan *et al*., Appl. Phys. Lett. **65**, 1466 (1994).

[7] M. Maldovan, Appl. Phys. Lett. **81**, 911 (2004).

[8] K. M. Ho, *et al*. *Solid State Commun*.89,413–416 (1994).