Enhanced Vertical Light Extraction From Ultrathin Amorphous Si–Si$_3$N$_4$ Multilayers With Photonic Crystal Patterns

Fang-Fang Ren, M. B. Yu, J. D. Ye, Q. Chen, G. Q. Lo, and D. L. Kwong, Fellow, IEEE

Abstract—We have investigated the significant enhancement of light extraction from amorphous Si–Si$_3$N$_4$ multiple-quantum-well structures, in which two-dimensional hexagonal-lattice air-hole photonic crystals (PCs) were integrated. The vertical spectral integrated intensity of light emission around 674 nm was enhanced up to $\sim 1.24$–$2.1$ times due to strong coupling to the inherent leaky modes or radiation modes near $\Gamma$ point of PC’s band structure. The experimental observations also suggested that coupling to leaky modes should be more beneficial for light extraction enhancement.

Index Terms—Light extraction, photoluminescence (PL), photonic crystal (PC).

I. INTRODUCTION

A n efficient Si-based light source could enable full monolithically integrated photonic circuits leveraging on Si-based complementary metal–oxide–semiconductor technology. Several materials have been investigated, exhibiting light emission in different spectral regions [1]–[4]. Previously, we have successfully demonstrated red light emission ($\lambda \sim 674 \text{ nm}$) from ultrathin amorphous Si ($\alpha$-Si)–Si$_3$N$_4$ multilayers [5]. However, the brightness was poor, mainly limited by the nature of Si indirect bandgap property.

It is well known that photonic crystal (PC) is capable of enhancing the light extraction [6]–[10] by providing a convenient way of redistributing the light energy in desired form and orientation, and also minimizing parasitic absorption in contrast with a randomly textured surface. As an alternative method to compensate the low internal quantum efficiency in Si-active materials, PC patterns have been widely utilized [11]–[13]. However, it is a lack of a multiple-quantum-well (MQW) structure integrated into PC patterns that is much closer to the design of a commercial light-emitting-diode device. In this study, we integrated two-dimensional (2-D) hexagonal-lattice air-hole PCs over the aforementioned ultrathin multilayer stack. The light extraction efficiencies were enhanced 1.24–2.1 times, consistent with the theoretical analysis.

II. EXPERIMENTAL DETAILS

Fig. 1(a) shows the schematic of the patterned sample. The multilayer stack consists of a 150-nm SiO$_2$ lower cladding layer, a 45-nm Si$_3$N$_4$ upper cladding layer, and a ten-period 3.0-nm $\alpha$-Si/9.0-nm Si$_3$N$_4$ MQW structure as the light-emitting active region. Fig. 1(b) shows the cross-sectional transmission electron micrograph (X-TEM) of the active layers. The detailed fabrication of the stack has been described elsewhere [5].

Subsequently, periodic hexagonal-lattice air-hole arrays were formed on the samples by dry etching with a fixed depth $h = 165 \text{ nm}$. After PC formation, all samples were subjected to post-deposition annealing at 700 °C for 30 min in nitrogen ambient to heal the etch damage and passivate the defect states [14].

In this work, two groups of PC patterns were fabricated and tested. The top-view images of scanning electron microscope (SEM) images for these patterns are shown in Fig. 2, and the detailed radius/lattice constant ($r/a$) are also labeled. Group-I...
includes patterns A and B with \( a = 400 \) nm, and group-II includes patterns C, D, and E with \( a = 700 \) nm. All air holes were designed to penetrate throughout the active region for the immediate consideration of concentrating the excitation energy inside the dielectric area, because the light tends to stay within the media with higher refractive index. As an example, Fig. 3(b) describes the normalized electric field distribution of the excitation light (\( \lambda = 325 \) nm) in the unit cell of numerical lattice of pattern A (\( r/a = 140/400 \) nm) in the plane of half etching depth. Fig. 3(a) is the corresponding geometry. It is found that the pump energy, which exhibits approximately hexagonal symmetry along six equivalent \( \Gamma \rightarrow M \) directions, mostly concentrates within the dielectric materials outside the air holes.

### III. RESULTS AND DISCUSSION

The samples were excited at room temperature using a He–Cd laser (325 nm) with the incident power of \( \sim 1.0 \) mW. The light emissions were collected by charged-coupled device system along the direction normal to the sample surface and the wavelength range was 400–1000 nm. Fig. 4 shows the photoluminescence (PL) spectra measured from the five patterned regions (A–E), as well as an unpatterned region for reference. Besides the obvious peak shifts modulated by the PC structures, the spectral integrated intensities were obtained \( \sim 1.24–2.1 \) times of enhancement over that without PC pattern. A similar enhancement (up to 4.49 times) has been reported by Makarova et al. in Si-based PC nanocavities due to a huge ratio of quality factor to mode volume \((Q/V)\) [11]. However, the enhancement in our work is based on coherent Bragg scattering by perfect periodic air-hole arrays. The different mechanism may be responsible for the difference in the improvement magnitude.

To gain better understanding on the experimental findings, we performed the calculation of band diagrams for the 2-D PC slabs based on the plane-wave expansion method and effective index theory. Since the thickness of each membrane stacked is much smaller than the emission wavelength, the multilayers are thus regarded as spatially homogenous medium with a lumped effective dielectric constant during the simulation.

Fig. 5(a) and (b) depicts the photonic band structures of patterns A (\( r/a = 140/400 \) nm) and B (\( r/a = 160/400 \) nm), respectively. Blue solid lines indicate the transverse-magnetic (TM)-like modes, and black dotted lines represent the transverse-electric-like modes. As shown in Fig. 4, the peak positions of patterns A and B appear around 663 and 635 nm, and accordingly, the values of normalized frequency \((a/\lambda)\) are estimated to be 0.6 and 0.63, respectively. These two values nearly refer to the TM-like radiation band at high-symmetry \( \Gamma \) point in the lattice reciprocal lattice, as marked in Fig. 5(a) and (b). It strongly suggests that the vertical extraction enhancement should be originated from strong coupling to the resonant radiation modes. Mathematically, the wave vector of modes can be expressed as \( \mathbf{k} = k_\parallel \mathbf{\hat{e}} + k_L \mathbf{\hat{e}}_L \), where \( k_\parallel (k_L) \) is the in-plane (out-plane) wave vector in the semiconductor. The modes lying below the escape cone are referring to guide modes \((k_\parallel > k_0)\), where \( k_0 \) is the in-plane wave vector in air, which are allowed to propagate in the horizontal plane, but will exponentially decay into the free space, analogous to the total internal reflection. However, the second-order TM-like band can be fold to resonant radiation band modes \((k_\parallel < k_0)\) at the Brillouin zone boundaries by phase compensation from a reciprocal lattice vector \( \pm G \), thus leading to higher external quantum efficiencies [15]. In addition, as compared with pattern A, the PL peak position of pattern B exhibits a visible blue-shift. The physics behind is the decrease of the effective refractive index of PC slab with the increasing radius.
strong coupling to the inherent leaky modes with high photonic density of state (DOS), i.e., low group velocity. To further confirm the dominant contribution of leaky modes, the band diagram of pattern C along the $\Gamma - M$ direction is shown in Fig. 6(a) from $a/\lambda = 0.9$ to 1.005 (640–778 nm), and the derived photonic DOS within the vicinity of $\Gamma$ point partly shown in Fig. 6(b). It is found that the PL peak around 650 nm ($a/\lambda = 1.077$) is very close to the $\Gamma$ point of the TM-like leaky bands, which exhibit maximal photonic DOS value around $a/\lambda = 1.076$. The emissions thus efficiently radiate into infinity along the vertical direction, in excellent agreement with the experimental observations in Fig. 4. Such consistencies also occur for patterns D and E.

In comparison, two interesting experimental findings in Fig. 4 could shed light on which pathway is more efficient for light extraction. First of all, for the patterns with the same filling factor $\rho$ (defined as $\tau/a$), such as A and D, or B and E, the PL intensities from group-II samples are much stronger than those from group-I, which indicates that the enhancement magnitude is strongly dependent on the lattice constant rather than the filling factor. Second, the best performance in group-II occurs at pattern E ($\tau/a = 280/700$ nm), for which the corresponding leaky modes have higher photonic DOS within the vicinity of $\Gamma$ point than the other patterns. All these facts imply that coupling to inherent leaky modes, especially with higher photonic DOS, should be more efficient for high external quantum efficiency rather than radiation modes.

Additionally, we can basically exclude the effect of surface/interface states on the improvement of luminescence quantum efficiency in this work. First, for instance, as compared to pattern E, pattern A has a more relative amount of top surface area ($\propto 1 - 2p^2/\sqrt{3}$) and inner surface area ($\propto 4\pi \rho p/\sqrt{3}a$), indicative of more surface/interface states involved. If these states are mainly responsible for the PL enhancement, pattern A should have higher PL intensity, but the experimental fact seems opposite. Moreover, as aforementioned, all patterned samples were annealed in nitrogen atmosphere and the defect states should be passivated greatly.

IV. CONCLUSION

In summary, perfect PC patterns are employed in ultrathin amorphous $\alpha$-Si–Si$_3$N$_4$ multilayers to enhance the light extraction. The spectral integrated PL intensities were achieved $\sim 1.24$–$2.1$ times of enhancement in the vertical direction, indicating strong coupling to resonant radiation or inherent leaky modes of PC patterns. The strongest enhancement occurring at pattern E shows that coupling to leaky modes with high photonic DOS should be more beneficial for light extraction improvement.

REFERENCES