Comparative analysis of void-containing and all-semiconductor 1.5 \( \mu \text{m} \) InP-based photonic crystal surface-emitting laser diodes

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ABSTRACT
This paper analyzes 2D photonic crystal surface-emitting laser diodes with void-containing and all-semiconductor structures by comparing their simulated mode distribution, band structure, and coupling coefficients. A photonic crystal design with a square lattice and circle atoms is considered.

I. INTRODUCTION
A photonic crystal surface-emitting laser (PCSEL) is a semiconductor laser in which a photonic crystal (PC) provides in-plane feedback and out-of-plane scattering. Laser oscillation occurs when light guided in-plane satisfies the second order Bragg diffraction condition, allowing large-area coherent emission. PCSELs have a number of desirable attributes, including single mode operation, low divergence, on-chip beam steering, Watt-class power, polarization and beam shape control, and coherently coupled arrays.

PCSELs were originally achieved by wafer fusion, but this method can result in discontinuities in the crystal lattice at the fusion interface inside the device, generating undesirable defect states. Epitaxial regrowth has the ability to overcome this issue and has been identified as a critical process to allow the realization of high power and high efficiency PCSELs. Depending on the growth conditions for epitaxial re-growth, voids or all-semiconductor PC structures can be selected. Void-containing PCSELs have been realized using metalorganic vapor phase epitaxy (MOVPE) in GaN materials at ~400 nm and GaAs at ~940 nm. We recently reported the realization of an InP-based epitaxially regrown PCSEL at 1.5 μm at room temperature, utilizing a void-containing PC. Similar structures operating at 1.3 μm have also been reported, as well as optically excited laser structures. These recent reports have provided a significant step in the development of InP-based PCSELs that may allow PCSEL technologies to find applications in areas such as high-speed optical communications, free-space communications, and LiDAR. A design analysis, comparing both void-containing and all-semiconductor InP-based PCSELs, is therefore highly needed.

Careful control of the MOVPE growth conditions allows the realization of either void-containing PC structures or all-semiconductor structures. Figures 1(a) and 1(c) show example cross-sectional TEM images of our re-grown all-semiconductor and void-containing InP photonic crystals, respectively. The corresponding schematic versions are shown in Figs. 1(b) and 1(d). Depending upon growth conditions, and the form of the etched structure prior to re-growth, either void-containing or all-semiconductor structures can be realized.

Engineering the PC shape allows control of out-of-plane coupling, but maximizing the in-plane coupling is critical to minimize loss of in-plane optical power. Figures 2(a) and 2(b) schematically illustrate the microscopic coupling mechanisms of a
square lattice PC layer, where $\kappa_3$ describes the light coupled in the forward and backward directions [Fig. 2(a)], with the coupling in the oblique in-plane directions represented as $\kappa_1$ [Fig. 2(b)]. The magnitudes of these coupling coefficients are governed by the index

\[ \kappa_i \text{ and } \kappa_d \text{ represent the incident and diffracted light waves, respectively.} \]  

\[ \kappa_i / \odot \llap{\vrule} \odot \llap{\vrule} \odot \llap{\vrule} \text{represents the coupling mechanism in the vertical directions.} \]  

\[ \alpha / \odot \llap{\vrule} \odot \llap{\vrule} \odot \llap{\vrule} \text{is the perpendicular radiation loss, and } \alpha \text{ is the in-plane radiation loss.} \]  

\[ \text{We note that the low refractive index PC layer tends to "push" the mode into the substrate.} \]  

\[ \text{Here, the PC region acts more like a waveguide, resulting in a strong mode overlap.} \]  

\[ \text{It has been pointed out that the low mode overlap but high refractive index contrast of the void-containing structures and the high overlap and lower refractive} \]
index contrast of all-semiconductor structures can result in similar coupling coefficients.\textsuperscript{11,23,24}

The method we apply to determine the in-plane coupling coefficients is to first determine effective mode-indices for the atom and field regions of the PC. These regions are shown schematically as dotted lines in Figs. 3(a) and 3(b). The calculated mode-indices are then used as the input to PWE simulations to determine the band-structure of the PC. The simulated PCSEL here is based on our five AlInGaAs multi-quantum wells design described in detail elsewhere.\textsuperscript{22} A circular atom shape is utilized (with an atomic radius \( r \) and period \( a \)), although this method is applicable to more complex shapes.\textsuperscript{2}

After determining the band structure, the coupling coefficients \( \kappa_3 \) and \( \kappa_1 \) can be further deduced from the coupled wave model outlined by Sakai \textit{et al.} from the following equations:\textsuperscript{21}

\[
\omega_{\text{CD}} = \frac{c}{n_{av}} \left( \beta_0 + \kappa_3 \right) \left( 1 - \frac{4\kappa_2^2}{\beta_0^2 - \kappa_3^2} \right), \tag{1}
\]
\[
\omega_{\text{B}} = \frac{c}{n_{av}} \left( \beta_0 - \kappa_3 \right), \tag{2}
\]
\[
\omega_{\text{A}} = \frac{c}{n_{av}} \left( \beta_0 - \kappa_3 \right) \left( 1 - \frac{4\kappa_2^2}{\beta_0^2 - \kappa_3^2} \right), \tag{3}
\]

where \( \omega_{\text{A, B, C, D}} \) are the normalized frequencies at each band edge, \( n_{av} \) is the average index of the PC, and \( \beta_0 = 2\pi/a \).

\section*{III. RESULTS AND DISCUSSION}

Figure 4(a) plots the calculated band structure for the all-semiconductor structure at 0.4 \( r/a \) over a limited range of the \( k \)-vector (0.2 X to 0.2 M). The inset shows the expanded regions near the \( \Gamma \) point to identify the degenerate and non-degenerate modes. The corresponding in-plane electric field distribution within the unit cell has also been indicated on the right side. Figure 4(b) is a similar plot but for 0.2 \( r/a \) with the void-containing structure. The symmetry of the electric fields demonstrates that the non-leaky modes appear at low frequencies with 0.2 \( r/a \) and shift to higher frequencies at 0.4 \( r/a \) and therefore the likely lasing modes. The higher refractive index contrast of the void-containing structure brings a larger bandgap at the \( \Gamma \) point in our device.

Figure 5 plots the normalized \( \Gamma \) point band frequencies for the four bands at various \( r/a \) values for all-semiconductor and void-containing structures. The non-degenerate band edges appear on the low frequency branch of the manifold at low values of \( r/a \). For \( r/a > 0.3 \), the non-degenerate branches are at higher frequency. The inset in Fig. 5 shows expanded plots of the band-structure in the region of the gamma point at 0.2 \( r/a \) and 0.4 \( r/a \) to illustrate the degenerate/non-degenerate character of the band edges under different structures. Beyond 0.5 \( r/a \) (not plotted), the circular patterns overlap, forming an apsamikkum, and at \( r/a \approx 0.7 \), the whole of the PC region is occupied by the atom. The general trend of band-edge frequency increasing with increasing \( r/a \) is due to the reduction in the average refractive index in the PC layer, reducing the overall mode index.

Figure 6(a) plots the absolute value of coupling coefficients \( \kappa_3 \) and \( \kappa_1 \), respectively, in both void-containing and all-semiconductor structures. These values were determined from the band-structure, as described in the Methods section.\textsuperscript{21} The corresponding calculated effective mode-indices are 3.244 \( (n_{\text{eff, A}}) \), 3.202 \( (n_{\text{eff, B}}) \), and 3.218 \( (n_{\text{eff, C}}) \). In both structures, the coupling coefficient \( \kappa_3 \) exhibits local maxima at \( r/a \approx 0.2 \) and global maxima at \( r/a \approx 0.45 \). \( \kappa_1 \) is observed to have a maximal value at \( 0.4 r/a \). The form of \( \kappa_3 \) forms a dual peak with zero at \( r/a \approx 0.3 \). The local maxima in \( \kappa_3 \) are at

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4}
\caption{Bandgap of the PC with the (a) all-semiconductor structure at 0.4 \( r/a \) and (b) void-containing structure at 0.2 \( r/a \). Black-arrows represent the direction of the electric field, and the their size represents the amplitude. The circle inside the electric field is the size of the PC atom in a unit cell.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5}
\caption{Photonic crystal band frequencies at the \( \Gamma \) point as a function of \( r/a \). The dotted line corresponds to the void-containing structure, and the solid line corresponds to the all-semiconductor structure.}
\end{figure}
r/a ~ 0.2 and ~0.45. At r/a = 0.2, we find $\kappa_3$ ($\kappa_1$) values of 88 (195) cm$^{-1}$ in all-semiconductor and 130 (288) cm$^{-1}$ in void-containing structures. This is an ~48% enhancement in both $\kappa_3$ and $\kappa_1$ at 0.2 r/a for void-containing structures. For the global maxima in $\kappa_3$ at r/a = 0.4, we find $\kappa_3$ ($\kappa_1$) values of 115 (495) cm$^{-1}$ in all-semiconductor and 168 (734) cm$^{-1}$ in void-containing structures, corresponding to an ~46% (~48%) enhancement by moving from an all-semiconductor to void-containing PC. Similar enhancement is obtained at r/a = 0.45.

Figure 6(b) plots the overlap of the lasing mode with the multi-quantum well elements calculated using an effective refractive index for the PC layer, as described in Fig. 3. The differential change in the mode overlap with r/a is also plotted to highlight how robust the device is to variations in PC manufacture. Similarly, Fig. 6(c) plots the normalized lasing frequency as a function of r/a, along with a differential. Regions of interest for PCSEL design (r/a $\sim$ 0.2 and ~0.4) are highlighted.

For r/a = 0.2, as discussed previously where a local maxima in $\kappa_3$ is observed, void-containing PC devices demonstrate higher coupling coefficients than all-semiconductor structures. In addition, a comparatively higher mode overlap with the quantum wells is observed (4.86% cf. 3.69%). This can be expected to be advantageous in modulation applications, reducing threshold current and heat, but may be disadvantageous for narrow spectral linewidth devices. We note that the rate of change of the mode overlap and frequency with r/a is higher in the case of void-containing PCs. This indicates that variation in the manufacturing process will result in larger variations in operating characteristics (wavelength, slope efficiency, and threshold current) for void-containing devices.

For r/a = 0.4, where $\kappa_1$ has a global maximum and $\kappa_3$ is close to its global maximum, again, void-containing structures demonstrate higher coupling coefficients. In this case, the all-semiconductor device has a higher mode overlap with the quantum well active element as the photonic crystal layer acts to “push” the mode into the substrate. In this case, the all-semiconductor structure shows a lower sensitivity of the mode overlap and lasing frequency to variations in r/a. This indicates that such structures may provide a “more manufacturable” device in terms of variation in the operating characteristics. The ease of mastering the epitaxial processes to achieving the control of semiconductor infill or void formation poses a different manufacturing challenge.

IV. CONCLUSIONS

A comparative simulation study of void-containing and all-semiconductor PCSELS with the square lattice and circle atoms has been presented. The variation in optical coupling coefficients, active element mode overlap, and lasing frequency with the radius of a circular PC atom have been discussed. Two regions of interest have been identified, and the relative merits of the two approaches for PC realization have been discussed. In general, a 0.2 r/a void-containing structure is suitable for modulation applications because of its related high mode overlap (4.86%). A 0.4 r/a void-containing structure is the choice for high power applications because of its high coupling coefficients in both $\kappa_3$ and $\kappa_1$ (168 and 734 cm$^{-1}$). Up to 50% of improvement in coupling can be achieved compared to that of an all-semiconductor structure. For minimal variation in device performance due to structural variation in the manufacturing process, an all-semiconductor structure with 0.4 r/a is the optimum choice.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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