Photonic band gap formation in silicon carbide triangular cross-section photonic crystals

Pranta Saha\textsuperscript{1}, Sridhar Majety\textsuperscript{1}, and Marina Radulaski\textsuperscript{1}

\textsuperscript{1}Department of Electrical and Computer Engineering, University of California, Davis, CA 95616, USA

Abstract

Triangular cross-section silicon carbide (SiC) color center photonics has recently emerged as a very promising platform for quantum information processing. Here, we investigate the dispersion relations in 1D SiC photonic crystals in triangular geometry and discuss the formation of photonic band gaps (PBGs). We compare the PBG formation trends and evaluate the fabrication suitability. Finally, we propose three distinct photonic device designs, resulting from unique PBG configurations, which are vital components for improving the efficiency of quantum photonic circuits.

1 Introduction

Formation of photonic band gaps (PBGs) in photonic crystals (PhCs) has been explored in the past three decades after the discovery made by Yablonovitch and John \cite{1,2}. Although wave propagation in periodic structures has almost been a century-long study \cite{3}, PhCs have gained attention due to their robust light confinement capability, scalability, and small footprint \cite{4,5}. Combination of different scatterers with unique lattice geometries \cite{6,16} has led to wider PBGs by reducing the structure symmetry and found applications in polarization beam splitters \cite{17,18}, optical logic gates \cite{19,20}, mirrors \cite{21,22}, sensors \cite{23,24}, lasers \cite{25,26}.

\textsuperscript{*}Corresponding author: prsaha@ucdavis.edu
solar cells \cite{27,28}, and more. Nevertheless, most of these studies have been conducted on either slab, rectangular, or cylindrical geometry.

Color centers are defects in single-crystal materials that can emit spin-entangled photons, upon excitation, which act as quantum information carriers. In recent times, photonics in triangular geometry has come into focus for increasing the efficiency of such solid-state quantum emitter processes \cite{29,32}. Triangular cross-section waveguide results from a bulk nanofabrication process called the angle-etch method that has been successfully implemented in both diamond \cite{29,33} and SiC \cite{30,31}. Previous fabrication processes were challenged by various imperfections that deteriorated the optical properties of the color centers or limited the robustness of the nanophotonic devices \cite{32}. On the other hand, triangular geometry offers emitter implantation in bulk substrates (free-standing waveguides), which ensures high-quality color centers with better coupling and can pave the way for efficient quantum photonic hardware.

Triangular cross-section PhCs have mostly been studied for constructing active photonic devices \cite{30,34,35} whereas the dispersion relations and PBG formations are yet to be discussed in detail. We shine a light on this issue to advance the photonic integration in color center based quantum devices. We choose SiC as an example host dielectric since it offers a collection of optically addressable color centers \cite{36} with long spin coherence times \cite{31,37,39}, excellent brightness \cite{40}, nuclear spins \cite{41,42}, and telecommunication wavelength emissions \cite{32,36} which are suitable properties for quantum information processing. On top of that, SiC has a large bandgap, high thermal conductivity, strong second-order nonlinearity, mechanical stability, and mature industrial presence \cite{12,15} making it a reliable platform to work with.

In this paper, we begin with defining the relevant parameters for analyzing PBG formation in SiC triangular cross-section PhCs. Using the plane wave expansion (PWE) method, we calculate the band structures and discuss the dispersion relations related to individual geometry. We then observe the effects of parameter variation on PBGs and examine the designs in terms of nanofabrication. We conclude by proposing three photonic devices along with their structural configurations and operational wavelength ranges which have the potential to be essential components of integrated photonic circuits.
2 Triangular cross-section photonic crystal

In this section, we define the parameters of the triangular cross-section photonic crystal. Traditionally, the periodic dielectric waveguides have periodicity along the direction of light propagation \( [43] \). The triangular cross-section PhC in this study is realized in a similar fashion. Our 1D PhC structure is designed by inserting cylindrical air holes along \( y \) axis in the SiC triangular cross-section waveguide as shown in Fig. 1(a). The most significant parameters of the PhC are its lattice constant \( a \), waveguide width \( w \), hole radius \( r \), and etch angle \( \alpha \). We examine three \( \alpha \) values 35°, 45°, and 60°, which fall under realistic fabrication parameters of the state-of-the-art processes [30,31,44]. We vary the width \( w \) from 1.2\( a \) to 2.25\( a \), and the radius \( r \) from 0.25\( a \) to 0.45\( a \). We consider the refractive index of SiC to be \( n_{\text{SiC}} = 2.6 \).

![Figure 1](image.png)

Figure 1: (a) Schematic of the 1D photonic crystal unit cell. (b) Electric field lines (arrow) associated with corresponding TE-like (red) and TM-like (blue) modes. (c) \( n_{\text{eff}} \) and VFF calculation as a function of \( r/a \) for \( \alpha = 45^\circ \).
Based on the existence of a mirror symmetry plane \((z = 0)\) perpendicular to the direction of periodicity, the photonic modes can be decoupled into transverse electric (TE-like) and transverse magnetic (TM-like) polarizations as illustrated in Fig. 1(b). Modes with electric field lines having odd symmetry about \(z = 0\) are TE-like as the electric field lies in the plane of propagation. On the other hand, TM-like modes have even symmetry at \(z = 0\) and the electric field lies in a direction perpendicular to propagation.

We use the effective refractive index \((n_{\text{eff}})\) as a useful parameter for understanding the modal profiles in a photonic device \([16,35,35]\). It is defined as the ratio of propagation constant \((\beta)\) of a mode to the vacuum wavenumber \((2\pi/\lambda)\). In triangular geometry, the TE/TM polarized modes supported by the structure propagate according to their corresponding \(n_{\text{eff}}\) values. Modes with lower \(n_{\text{eff}}\) are not well contained within the structure and become evanescent \([35]\). As guided modes depend on \(n_{\text{eff}}\), which is a strong function of the effective dielectric present in the photonic device, its value can help us interpret the dispersion relations and changes in PBGs due to parameter variation in the proposed 1D PhC. Hence, in the following, we come up with an analytical expression for estimated \(n_{\text{eff}}\) derived from the volumetric fill factor (VFF) of SiC in the PhC structure:

\[
    n_{\text{eff}} = \text{VFF} \times n_{\text{SiC}} + (1 - \text{VFF}) \times n_{\text{air}}
\]  

Fig. 1(c) demonstrates the changes in VFF and \(n_{\text{eff}}\) as a function of the normalized hole radii \((r/a)\) in the 45° angle-etched waveguide with various \(w\) values. The plots show that \(n_{\text{eff}}\) reduces for higher \(r/a\) and increases for higher \(w\). The latter happens due to the enlargement of the triangular cross-section with incremental \(w\) which leads to greater \(n_{\text{eff}}\) and more supported modes. We observe similar trends and values for 35° and 60°.

### 3 Dispersion relations in triangular geometry

While well studied in rectangular cross-section photonic crystals, the dispersion relations and PBG formations are not well understood in triangular geometry. Plane wave expansion (PWE) method has been widely used for analyzing PhCs due to its efficiency and accuracy
Figure 2: Dispersion relations for TE (red) and TM (blue) modes in the triangular cross-section 1D photonic crystal. The red (blue) shaded regions show the photonic band gaps for the TE (TM) modes. Parameters of the photonic crystal are: (a) $\alpha = 35^\circ$, $w = 1.2a$, $r = 0.35a$. (b) $\alpha = 45^\circ$, $w = 1.2a$, $r = 0.4a$. (c) $\alpha = 60^\circ$, $w = 1.35a$, $r = 0.43a$. 
in computing PBGs \cite{13,46,47}. It is a direct frequency eigensolver method, derived from Maxwell’s equations for a sourceless medium, where the eigenvalues are mode frequencies, and the eigenstates (plane wave solutions) are characterized by wavevector $k$ and a band number. The irreducible Brillouin zone, which contains allowed wavevectors with non-redundant mode frequencies, lies in the range of $(0,0,0)$ to $(0,\pi/a,0)$ in the $k$-space for 1D PhC according to our definition of periodicity \cite{48}. We have used MIT Photonic Bands (MPB) \cite{49} to employ the PWE method for investigating band structure and PBG formation in the above mentioned irreducible Brillouin zone of the triangular cross-section PhC.

The dispersion relations for three different PhC parameter sets ($\alpha, w, r$) are presented in Fig. 2. In the band structure, the first TE/TM band (dielectric band) is the fundamental mode with the fewest nodes and the lowest frequency. The fundamental mode is well guided by the structure in all three PhCs. However, the higher-order mode (air band) for TE/TM is not entirely guided due to the light line effect, and becomes more radiative with $\alpha$ getting larger, as depicted in Fig. 2. The TE (TM) PBG is formed by the range of frequencies present between the minima of the air band and the maxima of the dielectric band for the corresponding TE (TM) mode below the light line ($\omega < ck$). All three angle-etched 1D PhCs show both TE and TM band gaps. TE band gaps are larger than TM gaps due to the connected dielectric lattice structure which is in accordance with the general intuition \cite{50}. Fig. 2 also shows that 45° and 60° PhCs exhibit comparable TE gaps, while the 35° band gap is reduced. On the other hand, the TM gaps are comparable in 35° and 45° cases, and reduced for 60°.

Complete PBG refers to the region of forbidden propagation frequencies in the band structure regardless of polarization and is formed in the overlap of the TE and TM band gaps. Though conventional multilayered 1D PhCs lack a complete PBG \cite{51}, the triangular cross-section geometry offers complete PBG for all three studied angles $\alpha$. As PBG is the principal characteristic of a PhC, it is desired to obtain a design with as wide complete PBG as possible. Fig. 2 demonstrates that the largest complete PBG can be achieved with the 45° structure as the TM gap is completely buried within the TE gap. Complete PBG in the other two cross-sections occurs from a small overlapping region between the TE and TM band gaps. Even though in two ($w, r$) sets, the 60° geometry shows buried complete
Figure 3: (a)-(d) TE/TM photonic band gap in frequency \((c/a)\) and gap size \((\%\) w.r.t. normalized hole radii \((r/a)\) for the 45° triangular cross-section waveguide with \(w\) values of 1.2\(a\), 1.35\(a\), 1.5\(a\), and 1.75\(a\), respectively. In the frequency plots, the center points are midgap \((f_m)\) frequencies and the error bars indicate band widths \((\Delta f)\) for the corresponding TE/TM modes. The dashed circle shows the TE-TM gap overlap for the dispersion relations demonstrated in Fig. 2(b).
PBGs, these gaps are about four times narrower compared to the 45° case. Therefore, 45° angle-etched triangular cross-section 1D PhC is more favorable for polarization-independent light confinement.

4 Effects of parameters on PBG formation for $\alpha = 45^\circ$

In this section, we further analyze the effects of parameters to achieve the best performing design in the 45° angle-etched waveguide. Scale-invariant nature of Maxwell’s equations actuates the idea of presenting parameters and results in terms of lattice constant $a$. Consequently, the gap width $\Delta f$, where $f$ is frequency expressed in units of $c/a$, is not a useful measure to understand the extent of a PBG. The gap to midgap ratio ($\Delta f/f_m$), popularly known as the gap size, is a more telling characterization of the gap width as it is independent of the scaling. Fig. 3 manifests TE-TM gap ($c/a$) and gap size (%) variation with $r/a$ in $\alpha = 45^\circ$ waveguides having several widths $w$. With incremental $r/a$, the $n_{\text{eff}}$ decreases leading to an increase in $f_m$ for both the TE and TM band gaps, consistent with the literature [52]. The opposite happens when $w$ increases, due to the increased $n_{\text{eff}}$, for a corresponding $r/a$ value.

In smaller $w$ such as $1.2a$ and $1.35a$, the TE gap size initially increases with $r/a$ owing to fewer supported modes as a result of lower VFF and $n_{\text{eff}}$, but shrinks after reaching the resonant condition at which the gap size is maximum. This happens on account of the reduction in effective dielectric contrast with higher $r/a$ values. Apparently, TE gap size in PhCs with larger widths $w$ is smaller due to greater $n_{\text{eff}}$, and TE band gap vanishes above $w = 1.75a$. On the contrary, the TM gap size monotonically grows with $r/a$, however, the band gap disappears for larger widths, identical to the TE case. From Fig. 3 and the above discussion, it is evident that complete PBG (either buried or overlap) mostly occurs for smaller widths and TE/TM band gap totally vanishes for waveguides with larger widths ($w > 1.75a$).
5 Discussion

The demonstrated work provides insights into the dispersion relations in the non-standard, triangular, geometry of photonic crystals. Fig. 4 delineates a general comparison of TE/TM gap sizes among the three etch angles for a constant width \( w = 1.2a \). We observe that unique trend emerges from unique geometry. For the 35° triangular cross-section, the TE gap size appears stable with changes in hole radii, whereas the TM gap size variation is identical to the 45° case. On the other hand, the TE and TM gap sizes in the 60° geometry follow the same trend as the 45° TE case. In general, TE gaps in 35° and TM gaps in 60° cease to exist for PhCs with \( w > 1.5a \).

![Figure 4: TE/TM gap size (%) in \( w = 1.2a \) with varying normalized hole radii \( r/a \) for the three \( \alpha \) values.](image)

In addition to discussing the formation of photonic band gaps in photonic crystals with...
variation in parameters, it is imperative to evaluate the practicality and robustness of the designs in terms of fabrication. For instance, it is challenging to fabricate bigger holes \((r \geq 0.43a)\) in smaller widths \((w \leq 1.35a)\) because of the following two issues: i) there is \(\leq 18\%\) (of waveguide width \(w\)) space between the edge of the waveguide and the holes, and ii) only \(\leq 14\%\) (of unit cell \(a\)) room available between two adjacent holes. Therefore, a trade-off may need to be made deliberately, depending on the application, between the PBG size and the complexity of fabricating the device. Our recent work illustrates the design of a 60° angle-etched triangular cross-section 1D PhC mirror for enhancing the quantum efficiency of \textit{in situ} superconducting nanowire single photon detectors (SNSPDs) \[53\]. Even though 60° geometry does not provide the largest complete PBG, waveguide in this geometry supports single mode propagation for NV center emission in 4H-SiC which is essential for single photon detection as well as quantum communication \[54,55\].

Individual geometry offers distinct applications based on the PBG formation. We foresee three such applications from which integrated photonics with triangular geometry can benefit greatly. Operational ranges, discussed in the following, are calculated keeping a nominal wavelength of 1.1 \(\mu m\) at the midgap, suitable for divacancy light emission in 4H-SiC. First, one can make a TE-pass filter in the 1074 - 1124 nm range where the TM band gap forms in the 35° angle-etched waveguide with \((a, w, r) = (326, 570, 130)\) nm photonic crystal parameters. Second, the 60° triangular geometry with \((a, w, r) = (403, 705, 130)\) nm operates as a TM-pass filter from 1005 nm to 1214 nm where the TE band gap is formed. Third, a polarization-independent mirror can be constructed using the 45° waveguide with the parameters \((a, w, r) = (471, 565, 188)\) nm that provides complete PBG from 1078 nm to 1122 nm. The parameter features considered above are suitable for nanofabrication, and the wavelength ranges can also be scaled to fit wavelengths of other color centers by updating \(a\) which depends on the choice of the center wavelength of the band gap. Therefore, these designs have the potential to increase the efficiency of quantum photonic circuits.
6 Conclusion

Photonic integration of SiC color centers is known to enhance the efficiency of quantum hardware [56]. Here, the triangular geometry of devices can provide a combination of the pristine optical properties of the implanted color centers and the sample-agnostic nanofabrication. We have presented how photonic band gaps can be formed and applied in this geometry. As color centers have optical dipole-like emission, the exploration of the dispersion relations and PBG formations in triangular cross-section 1D PhCs can play a significant role for robust light confinement in quantum photonic hardware. Our simulated results show that the nature of PBG configurations primarily depends on the etch-angle and varies intuitively with other PhC parameters. The proposed three possible applications have the potential to improve the performance of integrated photonic devices with applications in quantum communication and quantum computing.

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Disclosures

The authors declare no conflicts of interest.

Data Availability Statement

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