Terms and Conditions of Use of Digitised Theses from Trinity College Library Dublin

Copyright statement

All material supplied by Trinity College Library is protected by copyright (under the Copyright and Related Rights Act, 2000 as amended) and other relevant Intellectual Property Rights. By accessing and using a Digitised Thesis from Trinity College Library you acknowledge that all Intellectual Property Rights in any Works supplied are the sole and exclusive property of the copyright and/or other IPR holder. Specific copyright holders may not be explicitly identified. Use of materials from other sources within a thesis should not be construed as a claim over them.

A non-exclusive, non-transferable licence is hereby granted to those using or reproducing, in whole or in part, the material for valid purposes, providing the copyright owners are acknowledged using the normal conventions. Where specific permission to use material is required, this is identified and such permission must be sought from the copyright holder or agency cited.

Liability statement

By using a Digitised Thesis, I accept that Trinity College Dublin bears no legal responsibility for the accuracy, legality or comprehensiveness of materials contained within the thesis, and that Trinity College Dublin accepts no liability for indirect, consequential, or incidental, damages or losses arising from use of the thesis for whatever reason. Information located in a thesis may be subject to specific use constraints, details of which may not be explicitly described. It is the responsibility of potential and actual users to be aware of such constraints and to abide by them. By making use of material from a digitised thesis, you accept these copyright and disclaimer provisions. Where it is brought to the attention of Trinity College Library that there may be a breach of copyright or other restraint, it is the policy to withdraw or take down access to a thesis while the issue is being resolved.

Access Agreement

By using a Digitised Thesis from Trinity College Library you are bound by the following Terms & Conditions. Please read them carefully.

I have read and I understand the following statement: All material supplied via a Digitised Thesis from Trinity College Library is protected by copyright and other intellectual property rights, and duplication or sale of all or part of any of a thesis is not permitted, except that material may be duplicated by you for your research use or for educational purposes in electronic or print form providing the copyright owners are acknowledged using the normal conventions. You must obtain permission for any other use. Electronic or print copies may not be offered, whether for sale or otherwise to anyone. This copy has been supplied on the understanding that it is copyright material and that no quotation from the thesis may be published without proper acknowledgement.
DESIGN, FABRICATION AND OPTICAL CHARACTERIZATION OF ONE-DIMENSIONAL TWO- AND MULTI-COMPONENT PHOTONIC CRYSTALS BASED ON SILICON

By

Anna Baldycheva

A thesis submitted to the University of Dublin for the degree of Doctor of Philosophy

Department of Electrical and Electronic Engineering
University of Dublin, Trinity College
Dublin
September, 2012
Declaration

I, the undersigned, declare that this thesis has not been submitted as an exercise for a degree in this or any other university or institution. The work described in this thesis is entirely my own, with exception of assistance recognized in the acknowledgments and the collaborative work noted in the publications. I furthermore agree that the Trinity College library may lend or copy this thesis on request.
Abstract

The objective of this thesis was the design, fabrication and optical investigation of a novel type of one-dimensional photonic crystal structures for application in integrated Silicon microphotonics. This thesis reports on new and unique optical properties of the developed ultra-wide pass-band filters based on multi-component photonic crystal model and thermo-, electro-tunable filters based on micro-cavity photonic crystal resonator model.

For the first time, the formation of the flat-top regions of transparency, pass-bands, was experimentally demonstrated for the grooved Silicon photonic crystal reflectors using the multi-component model. Using this method for the decrease of the optical contrast in photonic crystals allows omni-directional photonic band gaps to be obtained in high-contrast photonic crystal structures. The multi-component model enables easy and precise engineering of the optical contrast of the grooved-Silicon photonic crystal. This achieved, not by filling the air grooves with refractive index matching liquid, but via appropriate selection of the thickness or refractive index of the additional materials.

The proposed novel design of the electro-controllable band-pass integrated filters is based on the defect-free one-dimensional Silicon photonic crystal model and liquid crystal opto-fluidic technique, which allows the realization of the individual optical defects, microcavities, with tuning capabilities. By either varying the temperature or by application of electric field individually to each microcavity of the device the continuous precise tuning was demonstrated, which possess: i) the widest tunability of the resonance peaks known to date and ii) a unique fine electro-controllable tuneability of individual resonances in the system. Most importantly, only small change of the refractive index of liquid crystal is sufficient for realization of this tuning.

Finally, a model for investigation of the photonic band gap deviations caused by structural fluctuations in fabricated one-dimensional photonic crystals has been elaborated. It was established that the deviations of the photonic band gaps strongly depend on the magnitude of the structural fluctuations and increases with an increase in the order of the photonic band gaps. The approach has been proposed for the
determination of the fabrication tolerances and optimization of the photonic band gap properties of the fabricated photonics crystal structures.

The optical effects demonstrated have practical applications in integrated Silicon microphotonics. The models developed in this work can be applied to the design of one-dimensional photonic crystal devices of any micro- and nano-structured semiconductor or dielectric materials for application in optical-interconnects, biochemical sensing, medicine, defence and security across the entire electromagnetic spectrum.
Acknowledgements

As my thesis writing days draw to a close I would like to take this opportunity to thank those who made it all possible.

The research undertaken for this thesis was guided and encouraged throughout by Prof. Tatiana S. Perova, to whom I would like to express my gratitude and sincere appreciation for giving me the opportunity to embark on this exciting journey. I would like to deeply thank Prof. Perova for her time, encouragement and helpful discussions during all four years.

Prof. Vladimir Tolmachev for supplying guidance, help with writing of publications and many enlightening conversations during all these years and most of all for sharing his enthusiasm for research.

I would also like to thank all the past and present members of the Microelectronic Technology Group for all their help and interests, particularly, Elena Krutkova, Joanna Wasyluk, Sergey Dyakov, David Adley, Victor Ermakov, and Franz Schmied.

All collaborators, for their help with the sample fabrication and for many fruitful conversations along the way, particularly, Prof. Ekaterina Astrova, Dr. Yulia Zharova, Galina Li (Fedulova), Dr. Kevin Berwick and Dr. Mike Bain.

Prof. John Donegan’s and Prof. Louise Bradley’s group and especially Robert Lennox and Michael Lynch for help in building of experimental set-up and valuable discussions.

Part of the fabrication work was funded by Science Foundation Ireland through the National Access Programme (NAP) at Tyndall National Institute.

I would like to acknowledge all the engineers from Tyndall National Institute for the great fabrication job of the samples during NAP 94 and NAP 368, particularly people who did the really critical parts were Alan Blake, Brendan McCarthy (e-beam lithography), Jim Scully and Alan Hydes (Silicon-etch for the nano-structures).

I would like to acknowledge the full financial support from the ICGEE GREP (Internation School for Graduate Education in Nano- and Micro-Engineering), without which this work would not be possible. It was a great honor to get this award and to be a part of this great organization.
The Trinity Trust Travel Award for supporting financially travelling to the two major European Photonics conferences: SPIE Optical Metrology 2009 as a part of World of Photonics Congress 2009 in Munich and SPIE Photonics Europe 2012 in Brussels.

The SPIE Travel Award for supporting financially travelling to the SPIE Photonics Europe 2010 in Brussels.

To my mother for her love, support and patience and for always looking at the bright side of life. I love you mommy!

Finally, I would like to express my deepest appreciation to family and friends for all the laughs, good times and support through the PhD studies. Special thanks to aunty Nina, uncle Vova, aunty Anna, aunty Larisa, baba Ada, Mashulya, Ira, Masha, Anastasia, Elena, Julie, Camille, Misha, Marina, Pasha, Nina Sergeevna, Anya, Nadezhda Mikhailovna, Krolik, Milena. I am forever greatful for your friendship and understanding.
For my mother and
in memory of my grandparents.
# Table of Contents

*Declaration* .......................................................................................................................... ii  

*Abstract* .................................................................................................................................. iii  

*Acknowledgements* ................................................................................................................ v  

*Table of Contents* ................................................................................................................ viii  

*List of Figures* ....................................................................................................................... xi  

*Author’s Publications* ........................................................................................................ xxv  

*Chapter 1. Introduction* ........................................................................................................... 1  

1.1 Photonic Crystals ........................................................................................................ 2  

1.2 Si based Photonic Crystal devices ................................................................................ 4  

1.3 Tunable Photonic Crystal Devices ............................................................................. 9  

1.4 Photonic Crystals and their liquid crystal composites ............................................. 11  

1.5 Thesis Overview. .......................................................................................................... 12  

1.6 References ..................................................................................................................... 14  

*Chapter 2. Theoretical and Experimental Background* .................................................... 17  

2.1 Introduction ................................................................................................................... 17  

2.2 Calculation methods ..................................................................................................... 18  

2.2.1 The Transfer Matrix Method ............................................................................. 18  

2.2.2 Modelling of grooved Si structures .................................................................. 21  

2.2.3 Design of the Photonic Band Gap characteristics ........................................... 22  

2.2.4 Gap Map Approach ........................................................................................... 23  

2.3 Fabrication methods ..................................................................................................... 25  

2.3.1 Crystallographic Orientation of Silicon ........................................................... 25  

2.3.2 The Wet Anisotropic Etching Technique of (110) Si ...................................... 26  

2.3.3 The Deep Reactive Ion Etching Technique of (100) Si ................................. 29  

2.4 Methods of characterization ....................................................................................... 32
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.4.1 FTIR Microspectroscopy Technique</td>
<td>32</td>
</tr>
<tr>
<td>2.4.2 End-fire Technique</td>
<td>34</td>
</tr>
<tr>
<td>2.5 Summary</td>
<td>37</td>
</tr>
<tr>
<td>2.6 References</td>
<td>37</td>
</tr>
<tr>
<td>Chapter 3. Multi-Component Photonic Crystals</td>
<td>40</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>40</td>
</tr>
<tr>
<td>3.2 Fabrication methods</td>
<td>43</td>
</tr>
<tr>
<td>3.3 Model of Multi-Component Photonic Crystal Structure</td>
<td>45</td>
</tr>
<tr>
<td>3.3.1 Modelling of the additional regular layers</td>
<td>45</td>
</tr>
<tr>
<td>3.3.2 Gap Map presentation</td>
<td>46</td>
</tr>
<tr>
<td>3.4 Engineering of the optical contrast</td>
<td>48</td>
</tr>
<tr>
<td>3.4.1 Normal Incidence of Light</td>
<td>48</td>
</tr>
<tr>
<td>3.4.2 Oblique incidence of light: Omni-directional properties</td>
<td>55</td>
</tr>
<tr>
<td>3.5 Formation of Infrared Regions of Transparency</td>
<td>59</td>
</tr>
<tr>
<td>3.5.1 Suppression of Photonic Band Gaps</td>
<td>59</td>
</tr>
<tr>
<td>3.5.2 Influence of the additional component thickness</td>
<td>61</td>
</tr>
<tr>
<td>3.5.3 Influence of the oblique incidence of light</td>
<td>64</td>
</tr>
<tr>
<td>3.6 Photonic Crystal ultra-wide pass-band filter</td>
<td>67</td>
</tr>
<tr>
<td>3.7 Summary</td>
<td>72</td>
</tr>
<tr>
<td>3.8 References</td>
<td>73</td>
</tr>
<tr>
<td>Chapter 4. Micro-cavity Photonic Crystals</td>
<td>76</td>
</tr>
<tr>
<td>4.1 Introduction</td>
<td>76</td>
</tr>
<tr>
<td>4.2 Basic Concept: Modelling of 1D micro-cavity Photonic Crystals</td>
<td>77</td>
</tr>
<tr>
<td>4.3 Single cavity Photonic Crystal: a Fabry-Perot resonator</td>
<td>80</td>
</tr>
<tr>
<td>4.3.1 Gap Map design of Fabry-Perot resonators</td>
<td>80</td>
</tr>
<tr>
<td>4.3.2 Experimental: Fabrication and Optical Characterization</td>
<td>89</td>
</tr>
<tr>
<td>4.3.3 Ultra-wide tuning of resonance modes</td>
<td>97</td>
</tr>
</tbody>
</table>
List of Figures

Figure 1-1: On the right is the electromagnetic dispersion, with a forbidden gap at the wavevector of the periodicity. On the left is the electron wave dispersion typical of a direct-gap semiconductor, the dots representing electrons and holes. Since the photonic band gap straddles the electronic band edge, electron-hole recombination into photons is inhibited. The photons propagation is prohibited [6]. ...................................................................................................................................... 3

Figure 1-2: Simple examples of one-, two-, and three-dimensional photonic crystals. The different colors represent materials with different dielectric constants. The defining feature of a photonic crystal is the periodicity of material along one or more axes [3]. ......................................................................................................................... 4

Figure 1-3: SEM images of PhCs on Si platform: a) one-dimensional periodicity porous Silicon Bragg mirrors fabricated by vertical anisotropic etching of Silicon [12]; (b) two-dimensional hexagonal porous Si structure fabricated by anodization of p-type Silicon [12]; (c) three-dimensional Silicon photonic crystal woodpile structure fabricated by successive multiple masking-etching-alignment steps [13]. ........................................................................................................................................ 5

Figure 1-4: 2D-in-1D PhC waveguide for the measurements at 90° [18]....................... 6

Figure 1-5: a) Schematic structure of hollow waveguide; b) SEM image of cross-section of hollow waveguide [19]. ................................................................. 6

Figure 1-6: (a) SEM image of a Porous Silicon microcavity. (b) Resonance peak realized within the PBG at 0.63 nm [20]. ............................................................... 7

Figure 1-7: A point defect (cavity) realized in (a) macro-porous Silicon photonic crystal [16] and (b) in photonic crystal waveguide fabricated by X-ray lithography [21]. ................................................................................................................................. 8

Figure 1-8: (a) Optical image of the “fiber-photonic crystal-fiber” system; (b) Microresonators based on 1D PhC with defect; (c) Mirror based on 1D PhC [22]. ........................................................................................................................................ 8

Figure 1-9: Methods of active tuning (green) and correspondent parameters of tuning (blue) that can be realized in Si based Photonic Crystal devices ......................... 10
Figure 1-10: The nematic liquid crystal mesophase has an orientational order, but lacks of a long-range positional order, and exists between the crystalline and isotropic phases. \( \mathbf{N} \) is the nematic director [32].

Figure 2-1: Reflection, \( R \), and transmission, \( T \), of a plane wave by a multi-layer structure with high and low refractive indexes of layers. \( \Theta \) is the angle of incidence.

Figure 2-2: Schematic fragment of grooved-Si structure with (a) air grooves and (b) grooves infiltrated with LC.

Figure 2-3: (a) Calculations of the main PBG (1) and secondary PBGs (2, 3 etc.) for a 1D PhC based on the grooved Si with number of periods \( N=50 \), \( a=4\mu m \) at normal incidence of light. (b) Calculated reflectance spectrum of the structure with \( f_{Si}=0.226 \).

Figure 2-4: Planes defined by the Miller indexes.

Figure 2-5: Difference between (a, b) anisotropic and (c) isotropic wet etching [19].

Figure 2-6: (a) SEM image of Si walls for periodic photonic structure, obtained by deep anisotropic etching of (110) Si. (b) The optical microscopy image of 1D PhC, fabricated by WAE method: the top view of structure with lattice period \( a=7\mu m \).

Figure 2-7: Typical parallel-plate reactive ion etching system.

Figure 2-8: SEM images of the grooved-Si structures fabricated by DRIE: (a) The ARDE effect, (b) Bottling of the grooves, (c) Micrograss in the grooves, (d) Tilting of grooves [21].

Figure 2-9: Layout of a simple FTIR spectrometer.

Figure 2-10: (a, b) Schematic of the experimental set-up with IR beam focused by microscope on the grooved Si (position 1) and on bare Silicon (position 2). (c) Reflection characterization setup using a Fourier-transform infrared spectrometer coupled to an achromatic infrared microscope [25].

Figure 2-11: Schematic of the setup for end-fire light coupling using microscope objectives (also known as free-space coupling).

Figure 2-12: A free-space fiber coupling set-up. The insets demonstrate the light coupling using microscope objectives and in-plane alignment of the PhC sample during the optical measurements.
Figure 3-1: Schematic fragments of (a, b, c, e) two-component 1D PhC and (d) three-component 1D PhC with fixed value of lattice constant, a, and an additional t-layer. The thicknesses of H, L and t-layers are \(d_H, d_L, dt\), accordingly. 

Figure 3-2: Fabrication examples of the multi-component PhCs based on Si. Additional component obtained by a) thermal oxidation; b) stain etching; (c) infiltration with LC, and d) fabrication imperfection (here the corrugation of Si surface) as an additional t-layer.

Figure 3-3: a) The lowest stop-band regions for GMs of three-component 1D PhCs, obtained from a two-component PhC with optical contrast 3.42/1 (curve 1) with an additional regular t-layer with various thicknesses \(d_t\), shown, in units of a, by numbers beside the PBG areas. The value of \(n_t = 1.5\), number of periods \(N = 10\) and a normal incidence of light. For comparison, a two-component PhC with contrast 3.42/1.5, marked as 1.5, is also shown. The cutoff lines of the PBG regions correspond to \(\text{max}_{\text{FS}} = 0.74\) for \(d_t = 0.13a\), \(\text{max}_{\text{FS}} = 0.6\) for \(d_t = 0.2a\), \(\text{max}_{\text{FS}} = 0.46\) for \(d_t = 0.27a\), \(\text{max}_{\text{FS}} = 0.34\) for \(d_t = 0.33a\) and \(\text{max}_{\text{FS}} = 0.2\) for \(d_t = 0.4a\); b) Comparison of the lowest PBG areas for three-component and two-component PhCs with different optical contrasts (3.42/1, 3.42/1.1, 3.42/1.3 and 3.42/1.5), shown by numbers beside the curves.

Figure 3-4: Equivalency of the experimental PBGs of three-component PhCs with \(N = 4\), \(a = 4\mu\text{m}\) and \(f_{\text{Si}} = 0.157\) with additional layer thicknesses of the \(\text{SiO}_2\), \(d_{\text{SiO}_2} = 580\text{nm}\) and simulated PBGs of the same PhC without \(\text{SiO}_2\) component, but infiltrated with some unknown filler with refractive index \(n_f = 1.185\).

Figure 3-5: The dependence of \(n_{\text{Lequ}}\) (which is equivalent value for a two-component PhC) versus \(d/a\) for three-component PhC with a t-layer of thickness, \(d_t\), and refractive index, \(n_t\) (the numbers beside the lines) and \(f_{\text{Si}} = 0.2\).

Figure 3-6: Influence of the t-layer (\(d/a = 0.13a\)) on the shift and decrease of PBG regions of high order in the region \(N_F = 0-2.5\).

Figure 3-7: a) Gap maps of a two-component 1D PhC with contrast \(n = 3.42/1.5\) (curve 1.5) with added t-layers of different thicknesses \(d_t\), shown beside the curves in units of a, and with refractive index \(n_t = 2.2\). The GM with contrast \(n = 3.42/2.2\), the SB region marked as 2.2, is also presented for comparison. (b) Gap maps of a two-component 1D PhC with contrast \(n = 3.42/1.5\) (curve 1.5) with added t-layers of different thicknesses with a refractive index \(n_t = 1.7\). The GM with contrast
n=3.42/1.7, marked as 1.7, is presented for comparison. The calculation is performed at a normal incidence of light with the number of periods N=10. The cutoff lines are the same as in Figure 3-3. Note that only the lowest stop-band areas are shown for simplicity.

Figure 3-8: Transmission spectra shown for the lowest SB areas for a two-component PhC with an optical contrast of 3.42/1 (curve 1) and 3.42/1.5 (curve 1.5) and for three-component PhCs with an additional t-layer of ni=1.5 and thicknesses of dt=0.13a and 0.27a. Calculations were performed at a normal incidence of light with fsi=0.23 and N=10.

Figure 3-9: Gap maps, demonstrating the formation of an ODB region (the striped area), as a common area formed by the overlapping of PBG regions at different angles of incidence. Angles of incidence are indicated by the number beside the curves. The contrast was 3.42/1 and the additional layer had ni=1.5 and a) dt=0.2a, b) dt=0.27a, c) dt=0.33a and d) dt=0.4a. ODB regions for a two-component PhC with contrast of 3.42/1.5 (grey region) and for three-component PhC (striped region) are shown for comparison in (d).

Figure 3-10: The width of ODBs versus filling fraction (calculation from Figure 3-9).

Figure 3-11: Transmission spectra T and ODB width (filled rectangles) shown for the first PBG at incident angles of 0° and 85° for: a) three-component PhC (denoted as 3comp) with an additional layer ni=1.5 and dt=0.2a and two-component PhC (denoted as 2comp) with optical contrast 3.42/1 without ODB region (filling fraction fsi=0.3); b) three-component PhC with an additional layer ni=1.5 and dt=0.27a and two-component PhC with contrast 3.42/1.2 (fsi=0.3); c) three-component PhC with ni=1.5 and dt=0.33a, fsi=0.3 and two-component PhC with contrast 3.42/1.4 (fsi=0.3); d) three-component PhC with additional layer ni=1.5 and dt=0.4a and two-component PhC with contrast 3.42/1.5 (fsi=0.2). The dashed line corresponds to the level of Tpbg=0.001 (or Rpbg=0.999).

Figure 3-12: GMs for a two-component “Si-air” PhC (light regions) and for a multi-component PhC with ni=1.5 and dt=0.10a (dark regions) over a wide range of NF; maxfsi=0.8. The calculations are performed at normal incidence of light with number of periods N=5.

Figure 3-13: The transmission spectra T for multi-component PhC with t-layer refractive index ni=1.5 and thickness dt=0.10a for (a) fsi=0.08...0.1. (b) The same
as in figure (a) shown for clarity in expanded transmission scale for $f_{si}=0.087$. The calculations are performed at normal incidence of light with number of periods $N=5$.

Figure 3-14: a) The GM of stop-bands ($R>0.99$), denoted as SBs, and map of transmission bands ($T>0.99$), denoted as TBs, for the multi-component PhC with $n_i=1.5$ and $d_i=0.13a$. b) The transmission spectrum $T$ for the same multi-component PhC for $f_{si}=0.117$. The calculation is performed at normal incidence of light with number of periods $N=5$.

Figure 3-15: a) The GMs of PBGs (denoted as SBs) and maps of TBs (denoted as TBs) for the multi-component PhC with additional t-layer of refractive index of $n_i=1.5$ and thicknesses (a) $d_i=0.20a$ and (b) $d_i=0.33a$. The calculation is performed at normal incidence of light with number of periods $N=5$.

Figure 3-16: The GM of SBs ($R>0.99$) for TE-polarization (light regions) and map of TBs ($T>0.99$) for TM-polarization (dark regions) for the multi-component PhC with $d_i=0.2a$ in a wide $f_{si}$ range (a) and in limited $f_{si}$ range (b). The calculation is performed at angle of incidence $\theta=60^\circ$.

Figure 3-17: The T spectra for $f_{si}=0.18$ calculated for the multi-component PhC with $d_i=0.2a$ at angle of incidence $\theta=60^\circ$. The formation of TB for TM-polarization and SB for TE-polarization at NF=1.62 demonstrates the transformation of the PhC into TM-polarizer in transmission mode and TE-polarizer in reflection mode.

Figure 3-18: 3D representation of (a) flat-top SB centred at 0.8NF in the range of filling fractions $f_{si}=0.25-0.33$ before oxidation and (b) flat-top pass-band centred at the same frequency calculated for the same device after oxidation in the range $f_{si}=0.10-0.17$. The thickness of $SiO_2$ is $d_{SiO_2}=0.18a$.

Figure 3-19: (a) The GM of SBs with $R>0.99$ (light regions) and map of TBs with $T>0.99$ (dark regions) calculated for fabricated filter based on PhC structure (air-$SiO_2$-$Si$-$SiO_2$-air)$^N$ with $N=3$ for mid-IR. (b) The same maps, demonstrated in the limited range of $\lambda$ and $f_{si}$ for clarity. The dispersion of $SiO_2$ in MIR range and normal incidence of light $\theta=0^\circ$ are taken into account during calculations.

Figure 3-20: SEM image of photonic crystal filter based on grooved Si with thermally grown $SiO_2$ of thickness $d_{SiO_2}=0.72\mu m$. The lattice period $a=4\mu m$.

Figure 3-21: Experimental (dashed line) and calculated (solid line) (a) $R$ and (b) $T$ spectra of the band-pass filter based on PhC structure (air-$SiO_2$-$Si$-$SiO_2$-air)$^N$ with
N=3 demonstrate the transformation of the SBs at 3.5 μm and at 4.8μm into the TB at the wavelength λc = 4.2 μm.

Figure 4-1: Schematic fragments of (a) defect-free 1D PhC and 1D PhCs with (c) single and (e) triple optical defects. (b, d, f) The TMM simulated reflection spectra for the sixth order SB are demonstrated in normalized wavelength units NW=λ/a ((b) lower scale) and normalized frequency NF=ν/λ ((b) upper scale). The value of filling fraction is 0.243 and the refractive index of defect is $n_{cav1, 2, 3}=1.5$ (light green line) or $n_{cav1, 2, 3}=2$ (black line). R spectra of the single 1.5 periods FPRs are also shown for comparison (dashed lines).

Figure 4-2: (a) Map of stop-bands (shown by red contour with symbolic numeration) with R>0.85 and regions of transparency (black contour) with T>0.99 for 1.5-period PhC or FPR (shown in insertion). The incoming and outgoing media are air, $n_S=3.42$, and the incidence of light is normal. (b) The R spectrum for $f_S=0.11$ with few largely-modulated resonance peaks between SBs 1a-1b, 2c-2d and 2d-2e. (c) Spectrum R for $f_S=0.4$ demonstrated the absence of narrow resonance peak between SBs 1a-2a, 3b-4b.

Figure 4-3: (a) The map of stop-bands (oval-like figures) and transmission bands (lines) for 1.5-period PhC (FPR) based on 3-layers model “Si-LC-Si” with two values of $n_{LC}=n_1=1.49$ (red contours for SBs and pink lines for TBs) and $n_{LC}=n_2=1.69$ (black contours for SBs and grey lines for TBs). $R_{cutoff}=0.85$, $T_{cutoff}=0.99$. (b) Spectrum R calculated for $f_S=0.06$ and demonstrating the cut off line of R values, used for drawing of SBs map. (c) Fine tuning of peak positions and stop-bands with variation of $n_{LC}$ from 1.49 to 1.69. Relative peak shift $ΔNF/NF=0.14/1.33=10.5%$.

Figure 4-4: (a) The map of SBs for 3-period PhC “Si-air” (black contour) and 3-period PhC “Si-air” with LC “optical” defect (red contour) with $n_{LC}=1.49$.

Figure 4-5: R spectra for $f_S=0.15$ (b), 0.4 (c) and 0.6 (d) (see GM in Figure 4-4)

Figure 4-6: The map of SBs for 3-period PhC “Si-LC” with $n_{LC}=1.49$ (red contour) and map of TBs (black lines)

Figure 4-7: (a) The map of stop-bands ($R_{cutoff}=0.85$) for 3-period PhC “Si-LC” (see insertion) with tunable LC optical defect at $n_{LC}=1.49$ (red contours) and 1.69 (black contours). (b) Reflection spectra, R for $f_S=0.05$ with $n_{LC}=1.49$ (red line)
and 1.69 (black line); (c) the extended transmission spectra, T, with relative peak shift of $\Delta NF/NF = 9.7\%$ for SB 1c.

Figure 4-8: SEM images of air-resonator, fabricated on SOI platform, using (110)Si, with (a) reservoir for LC infiltration and b) the cross-section of the resonator edge. Depth of Si-walls is $h_{Si}=20\mu m$.

Figure 4-9: Schematic presentation of Fabry-Pérot resonator, consisting of two Si walls separated by (a) a gap and infiltrated with liquid crystal molecules with different alignment: (b) vertical planar, (c) horizontal planar, (d) isotropic, (e) homeotropic and (f) horizontal planar with air voids.

Figure 4-10: The (a) experimental and (b) calculated reflection spectra for air (dashed line) and LC (solid line) resonators. For spectrum, shown in (b), $n_{cm}=1$ (dashed line) and $n_{LC}=1.72$ (solid line) for $d_{Si}=1.2 \mu m$ and $d_{cav}=3.4\mu m$. The height of Si wall is $h_{Si}=50\mu m$.

Figure 4-11: The (a) experimental and (b) calculated reflection spectra for LC-resonator for $E$-(solid line) and $H$-polarization (dashed line). Calculated spectra with $n_{LC}=1.72$ (solid line) and $n_{LC}=1.53$ (dashed line), $d_{Si}=1.2\mu m$ and $d_{cav}=3.4\mu m$.

Figure 4-12: The (a) experimental and (b) calculated reflection spectra in NIR range vs. wavelengths (from Figure 4-10).

Figure 4-13: The (a, b) experimental reflection $H$-spectra of empty (dashed line) and LC (solid line) resonator vs. (a, c) wavenumber and (b, d) wavelength. (c, d) Calculated spectra with $n=1$ (dashed line) and $n_{LC}=1.53$ (solid line). SEM images of the resonator: (e) the top view and (g) a sidewall roughness, obtained after DRIE of (100)Si, $h_{Si}=20\mu m$.

Figure 4-14: (a, c) The experimental reflection spectra of LC resonator, demonstrated the effect of thermo-tuning, namely the transition from LC mesophase at 20 °C (dashed line for $H$- and thin line for $E$-polarization) to the isotropic phase at 65 °C (thick line). (b, d) Calculated spectra with $n_{LC}=1.67$ (thin line), $n_{LC}=1.54$ (thick line) and $n_{LC}=1.5$ (dashed line). $d_{cav}=3.6 \mu m$, $d_{Si}=1.2 \mu m$ and $h_{Si}=50 \mu m$.

Figure 4-15: SEM image of the top view of the FPR fabricated on an SOI wafer.

Figure 4-16: FTIR (a) reflection and (b) transmission spectra of the FP resonator with LC filler for $E$-(thick line) and $H$-(thin line) polarizations in the absence of an
applied electric field. The resonator parameters are: width of Si walls, \(d_{Si}=1 \text{ \mu m}\), cavity width, \(d_{cav}=4 \text{ \mu m}\).

Figure 4-17: Experimental (a) reflection and (c) transmission spectra in E-polarization in the absence (0V - thin line) and presence (10V thick line) of an applied electric field. The spectral shift observed demonstrates the reorientation of LC molecules in the FP-cavity from planar to homeotropic alignment. b) Calculated reflection spectra, obtained from the best fit, for two values of \(n_{cav}\) shown beside the curves. Resonance peaks are seen at 1800, 2320 and 3400 cm\(^{-1}\), corresponding to 5.6, 4.2 and 2.9 \text{ \mu m}.

Figure 4-18: Smooth tuning of the position of the resonance peak from 3330 cm\(^{-1}\) to 3550 cm\(^{-1}\) for E- and H-polarization (dotted line). The applied voltage is shown in Volts beside each curve.

Figure 4-19: (a) Experimental and (b) calculated E-polarized spectra of the FP resonator with \(d_{Si}=0.6 \text{ \mu m}\) and \(d_{cav}=7.4 \text{ \mu m}\) without electric field (thin line) and with an electric field generated by an applied voltage of 15 V (thick line). Application of a voltage of 15 V results in a shift of the resonance peaks across the spectral range. The best fit is obtained at \(\Delta n_{LC} = 0.17\) (\(n_{LC} = 1.51, 0\text{ V}\)) and \(n_{LC} = 1.34, 15\text{ V}\).

Figure 4-20: Smooth tuning of the resonance peak from 1700 to 1880 cm\(^{-1}\) in the experimental reflection spectra of the FP resonator (from Figure 4-17) with a maximal relative shift of \(\Delta \lambda / \lambda = 10\%\).

Figure 4-21: (a) Schematic view on the variation of the refractive index of LC E7 in the cavity under an applied voltage \(V\) (see Section 4.3). (b, c) The controlled variation of the \(n_{cav}(1), n_{cav}(2), n_{cav}(3)\) that can be realized in triple-cavity system.

Figure 4-22: (a) The GM of Si 1D PhC with a triple cavity with \(n_{cav}(i)=n_{cav}(1)=n_{cav}(2)=n_{cav}(3)=1.63\) in a wide range of NW. The triple resonances within the first order SB calculated for (b) \(f_{Si}=0.1\), (c) \(f_{Si}=0.2\), (d) \(f_{Si}=0.3\) and \(a=573\text{ nm}\). The estimated channel spacing, \(\lambda_{S1,2,3}\), and FWHM of each individual resonance are also demonstrated.

Figure 4-23: (a) The cavity refractive indexes \(n_{cav}(1,2,3)\) versus relative channel position shift normalized to the original channel spacing. (b) Continues tuning of the central channel for \(\Delta n=-0.026\) (red dashed line), \(\Delta n=-0.013\) (red dashed dotted line), \(\Delta n=0\) (black line), \(\Delta n=0.013\) (thin blue line) and \(\Delta n=0.026\) (thick...
blue line). (c) The GM of T=100%, calculated for Δn=−0.026 (red dashed line) and
Δn=+0.026 (blue line). Optimal design region is shown by ellipse. 114

Figure 4-24: (a) The cavity refractive indexes $n_{cav}(1,2,3)$ versus the ratio of the
channel spacings, $\lambda_{12}/\lambda_{13}$. (b) Continues blue shift of the edge channels with linear
decrease of the central cavity refractive index,$n_{cav}(2)$, by, $Δn=0.02$ (thin black line), $Δn=0.052$ (dashed blue line), $Δn=0.11$ (dashed dotted blue line). The triple
channels, for $Δn=0$, are also demonstrated (thick black line). (c) Continues red
shift of the edge transmission channels with linear increase of the central cavity
refractive index,$n_{cav}(2)$, by, $Δn=0.02$ (thin black line), $Δn=0.052$ (red dashed line), $Δn=0.11$ (red dashed dotted line). (d) The GM of $T=100\%$, calculated for
$Δn=−0.052$ (blue line) and $Δn=+0.052$ (red dashed line). .......................... 117

Figure 4-25: (a) The cavity refractive indexes $n_{cav}(1,2,3)$ versus the edge channel
intensity $I_{1,3}$ normalized to the maximum original intensity $I_0=I_2$ (lower scale) and
versus the relative channel spacing shift normalized to the original channel
spacing (upper scale). (b) The precise attenuation of the edge channel intensities,
$I_{1,3}$ for $Δn=0.015$ (red line), $Δn=0.03$ (green line), $Δn=0.05$ (blue line), $Δn=0.07$ (cyan line) demonstrated for the $f_{Si}=0.2$. (c) The GM of $T=25-100\%$, calculated
for $Δn=0.06$. (d) The attenuation of the edge channels for $Δn=0.06$ and $f_{Si}=0.35$.
(e) Fine attenuation from 100 % to 90 % for $Δn=0.005$ (red line), 0.01 (green line), 0.015 (blue line) demonstrated for the $f_{Si}=0.2$. ......................... 119

Figure 4-26: (a) The SOI-based chip design of the triple-coupled defect photonic
crystal filter filled with nematic LC (green colour) and metal contact pads (yellow
circles). (b) SEM image of the fabricated defect-free 1D PhC with three-channels
connected to 2nd, 4th and 6th grooves. (c) SEM image showing a view on the
channels from the cone-shape cavity designed for LC infiltration. ...................... 120

Figure 4-27: (a) SEM image demonstrates the structural deviations obtained for the
defect-free 1D PhC with $a=900$ nm, $f_{Si}=0.4$. (b) Transmission spectra of the
originally designed triple-defect device (black line) and of the fabricated device
with structural deviations of ±$δ d_{Si}=20$ nm (red line). The refractive index of all
cavities $n_{cav}(1,2,3)=1.63$. (c) A precise adjustment of the edge channels by
decreasing the refractive index to $n_{cav}(1,2,3)=1.60$. (d) Final adjustment of the
central channel with $Δn=0.01$. ................................................................. 121
Figure 5-1: Schematic diagram of a seven-period, 1D PhC with a lattice constant $a=d_H+d_L$ and an optical contrast of $n_H/n_i$. A wall thickness with fluctuation $(d_{j_H})$ in the H-component appears in each lattice period, causing a variation $(d_{j_L})$ in the L-component of the structure.

Figure 5-2: (a), (b), (c) R and (d), (e), (f) T spectra of an ordered PhC based on a "Si-air" structure for (a),(d) $f_H=0.23$; (b, e) $f_H=0.5$ and (c, f) $f_H=0.08$. The number of lattice periods, $N=7$, the incoming and outgoing medium is air and a normal incidence of light is used for these calculations. The numbers correspond to the order number of the PBGs from Figure 5-3.

Figure 5-3: Gap Map for ordered PhC, based on "Si-air" structure, with $N=7$. The lines, intersecting the PBG regions labelled with the numbers shown, are demonstrated for $f_H =0.23$ (dashed line), $f_H =0.08$ (dotted line) and 0.5 (short dotted line).

Figure 5-4: Histograms for 12 types of thickness fluctuation distribution values $\delta$, for an eight wall PhC with standard fluctuation $\delta=0.05$.

Figure 5-5: Gap maps of an a) ordered (thin line) PhC (from Figure 5-3) and a disordered (thick line) PhC with standard random thickness deviation of the walls of $\delta=0.05$. The fluctuation distribution used is type 1 from Figure 5-4(a), (b) Gap maps under identical conditions to those in figure (a) but with fluctuation distribution of type 8 (Figure 5-4(h)) and (c) type 6 (Figure 5-4(f)). Wall fluctuations are proportional to wall thickness. The dashed line corresponds to $f_H=0.23$ and the dotted lines correspond to $f_H =0.08$, 0.5 and 0.71.

Figure 5-6: Transmission spectra T for ordered (black line) and disordered (grey line) PhCs with filling fractions a) $f_H =0.08$, b) 0.23, c) 0.5, d) 0.71, with corresponding thickness fluctuations $\delta d_H = 0.004a$, 0.0115a, 0.025a and 0.036a and fluctuation distributions of type 1 from Figure 5-4(a) and Table 5-1. Numbers inside the dips (PBGs) correspond to the number of the PBG shown on the gap map in Figure 5-5(a).

Figure 5-7: T spectra for ordered (black line) and disordered (grey line) PhC with fluctuation distribution of type 8 for a) $f_H=0.23$ and b) $f_H=0.5$ with thickness fluctuations $\delta d_H = 0.0115a$ and 0.025a, respectively.

Figure 5-8: T spectra for ordered (black line) and disordered (grey line) PhCs with filling fractions of a) $f_H=0.23$, b) $f_H=0.5$ with corresponding thickness fluctuations.
\[ \delta d_H = 0.0115a \text{ and } 0.025a. \] The fluctuation distribution of type 6 from Figure 5-4(f) was used.

**Figure 5-9:** Gap map of ordered (black line) and disordered (grey line) PhC with a standard deviation in thickness \( \delta = 0.2 \) and fluctuation distribution of type a) 1 and b) 6. The value of the fluctuation \( \delta d_H = 0.016a \) is constant for different wall thicknesses.

**Figure 5-10:** T spectra of ordered (black line) and disordered (grey line) PhC with fluctuations of type 1 for a) \( f_H = 0.08 \), b) \( f_H = 0.23 \), c) \( f_H = 0.5 \) and d) \( f_H = 0.71 \). The value of the thickness fluctuation \( \delta d_H = 0.016a \) is constant for different wall thicknesses.

**Figure 5-11:** T spectra of ordered (black line) and disordered (grey line) PhC with fluctuation distribution of type 6 for a) \( f_H = 0.08 \), b) \( f_H = 0.23 \), c) \( f_H = 0.5 \) and d) \( f_H = 0.71 \). The value of the thickness fluctuation \( \delta d_H = 0.016a \) is constant for different wall thicknesses.
# Acronyms and Abbreviations

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>BD</td>
<td>Band diagram</td>
</tr>
<tr>
<td>BOX</td>
<td>Buried Oxide</td>
</tr>
<tr>
<td>CMOS</td>
<td>Complementary metal oxide semiconductor</td>
</tr>
<tr>
<td>DRIE</td>
<td>Deep reactive ion etching</td>
</tr>
<tr>
<td>FP</td>
<td>Fabry-Perot</td>
</tr>
<tr>
<td>FPR</td>
<td>Fabry-Perot resonator</td>
</tr>
<tr>
<td>FSR</td>
<td>Free spectral range</td>
</tr>
<tr>
<td>FTIR</td>
<td>Fourier transform infrared</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full width at half maximum</td>
</tr>
<tr>
<td>GM</td>
<td>Gap Maps</td>
</tr>
<tr>
<td>IB</td>
<td>Interference bands</td>
</tr>
<tr>
<td>LC</td>
<td>Liquid crystal</td>
</tr>
<tr>
<td>MEMS</td>
<td>Microelectromechanical systems</td>
</tr>
<tr>
<td>MIR</td>
<td>Middle infrared</td>
</tr>
<tr>
<td>NF</td>
<td>Normalized frequency</td>
</tr>
<tr>
<td>NIR</td>
<td>Near infrared</td>
</tr>
<tr>
<td>NW</td>
<td>Normalized wavelength</td>
</tr>
<tr>
<td>ODB</td>
<td>Omni-directional band</td>
</tr>
<tr>
<td>PB</td>
<td>Pass band</td>
</tr>
<tr>
<td>PBG</td>
<td>Photonic band gap</td>
</tr>
<tr>
<td>PhC</td>
<td>Photonic crystal</td>
</tr>
<tr>
<td>RIE</td>
<td>Reactive ion etching</td>
</tr>
<tr>
<td>SB</td>
<td>Stop band</td>
</tr>
<tr>
<td>TB</td>
<td>Transmission band</td>
</tr>
<tr>
<td>TE</td>
<td>Transverse electrical</td>
</tr>
<tr>
<td>TM</td>
<td>Transverse magnetic</td>
</tr>
<tr>
<td>TMM</td>
<td>Transfer matrix method</td>
</tr>
<tr>
<td>$a$</td>
<td>Lattice constant</td>
</tr>
<tr>
<td>$d_{\text{air}}$</td>
<td>Thickness of air component</td>
</tr>
<tr>
<td>$d_{\text{cav}}$</td>
<td>Thickness of cavity</td>
</tr>
<tr>
<td>$d_l$</td>
<td>Thickness of high-refractive index component</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>((d_{HI})_i)</td>
<td>Thickness of the (i)-th high-refractive index component</td>
</tr>
<tr>
<td>(d_L)</td>
<td>Thickness of low-refractive index component</td>
</tr>
<tr>
<td>((d_{LI})_i)</td>
<td>Thickness of the (i)-th low-refractive index component</td>
</tr>
<tr>
<td>(d_{Si})</td>
<td>Thickness of Si component (Si wall)</td>
</tr>
<tr>
<td>(d_{SiO_2})</td>
<td>Thickness of SiO(_2) component</td>
</tr>
<tr>
<td>(d_t)</td>
<td>Thickness of additional (t)-layer</td>
</tr>
<tr>
<td>(f_H)</td>
<td>Filling fraction of high-refractive index component</td>
</tr>
<tr>
<td>((f_{HI})_{\text{min}})</td>
<td>Minimum level of high-refractive index component filling fraction</td>
</tr>
<tr>
<td>(f_L)</td>
<td>Filling fraction of low-refractive index component</td>
</tr>
<tr>
<td>(f_{Si})</td>
<td>Filling fraction of Silicon</td>
</tr>
<tr>
<td>(h_{Si})</td>
<td>Etching depth of Silicon walls</td>
</tr>
<tr>
<td>(I)</td>
<td>Intensity</td>
</tr>
<tr>
<td>(i)</td>
<td>Number of the high-refractive index component</td>
</tr>
<tr>
<td>(N)</td>
<td>Number of periods</td>
</tr>
<tr>
<td>(n_{air})</td>
<td>Refractive index of air component</td>
</tr>
<tr>
<td>(n_e)</td>
<td>Extraordinary refractive index of LC</td>
</tr>
<tr>
<td>(n_{E7})</td>
<td>Refractive index of nematic liquid crystal E7</td>
</tr>
<tr>
<td>(n_H)</td>
<td>Refractive index of high-refractive index component</td>
</tr>
<tr>
<td>(n_{L})</td>
<td>Refractive index of low-refractive index component</td>
</tr>
<tr>
<td>(n_o)</td>
<td>Ordinary refractive index of LC</td>
</tr>
<tr>
<td>(n_{rand})</td>
<td>Refractive index value for a random orientation of the LC molecules</td>
</tr>
<tr>
<td>(n_{Si})</td>
<td>Refractive index of Silicon layer</td>
</tr>
<tr>
<td>(n_{SiO_2})</td>
<td>Refractive index of SiO(_2) layer</td>
</tr>
<tr>
<td>(n_t)</td>
<td>Refractive index of (t)-layer</td>
</tr>
<tr>
<td>(m)</td>
<td>Order of reflection band/transmission band</td>
</tr>
<tr>
<td>(max_{Si})</td>
<td>Maximum value of filling fraction of Si component</td>
</tr>
<tr>
<td>(por_{Si})</td>
<td>Porous Silicon</td>
</tr>
<tr>
<td>(Q)</td>
<td>Quality factor</td>
</tr>
<tr>
<td>(R_{PBG})</td>
<td>Minimum reflection level of photonic band gap</td>
</tr>
<tr>
<td>(R_{cutoff})</td>
<td>Reflection cutoff level</td>
</tr>
<tr>
<td>(T_{PBG})</td>
<td>Maximum transmission level of photonic band gap</td>
</tr>
<tr>
<td>(T_{cutoff})</td>
<td>Transmission cutoff level</td>
</tr>
<tr>
<td>(V)</td>
<td>Voltage</td>
</tr>
</tbody>
</table>
\( \Delta d_{II} \) Thickness deviation range of high-refractive index component
\( \Delta f \) Range of filling fraction
\( \Delta N F_{O D B} \) Width of omni-directional reflection band in normalized frequency
\( \Delta n \) Refractive index change
\( \Delta n_{E7} \) Refractive index change of nematic liquid crystal E7
\( \Delta n_{LC} \) Birefringence of LC
\( \Delta R \) Reflection signal modulation
\( \delta \) Standard deviation
\( \delta_i \) Relative deviation of the \( i \)-th high-refractive index component
\( \delta d \) Thickness deviation
\( \delta d_{II} \) Thickness fluctuation of the \( i \)-th high-refractive index component
\( \delta f_{Si} \) Step size of Silicon filling fraction range
\( \theta \) Angle of incidence of light
\( \lambda_c \) Band-pass filter wavelength of operation
\( \lambda_m \) Stop band/pas band operational wavelength
\( \lambda_s \) Channel spacing
Author’s Publications

Peer-Reviewed Publications


**Conference Proceedings**


7. A. V. Baldycheva, V. A. Tolmachev and T. S. Perova, Influence of geometrical dimensions fluctuations on photonic band gap regions for one-dimensional silicon


15. S. Dyakov, E. Astrova, V. Tolmachev, G. Fedulova, T. Perova, A. Baldycheva, V. Timoshenko, S. Tikhodeev and N. Gippius, Optical spectra of two-dimensional


xxviii


Chapter 1.

Introduction

It is now one-half century since the advent of the solid state electronics with the invention of the transistor. The semiconductor revolution, which is still continuing, enabled profound and unanticipated improvements in our standard of living. Advances in semiconductor physics have had a profound impact on all aspects of society transforming the way people work, live, learn and communicate [1]. The resultant explosion in information technology is based on the ability to control the flow of electrons in a semiconductor in the most intricate ways.

What is known today as a technology shrink has increased computational speed due to a shorter gate width, increased functionality through higher levels of integration and decreased costs by processing more transistors/chip and more chips/wafer. The key driving forces for the Silicon electronics technology roadmap is a high speed and functionality at low cost. In the last three decades, this performance level has increased exponentially with rates of more than 100/decade. This has led to increasingly difficult problems in communication between computer boards, chips and even individual chip components as well as the integration of optics and microelectronics. These problems create an interconnect bottleneck which is a 'grand challenge' to be overcome by the semiconductor industry according to the ITRS (International Technology Roadmap for Semiconductors).

The invention of the laser in the nineteen sixties inspired the photonics industry, thus enhancing the transmission of information by replacing electronic signals in wires with laser pulses in optical fibres. The alternative interconnect technology can be Silicon based optical interconnects, which can efficiently deal with large bandwidths of information and is not limited by resistance, capacitance and reliability constraints of metal lines. In particular, the incorporation of optical components on a Silicon chip
would provide a new platform for the monolithic integration of optics and microelectronics and open doors to new technologies. However, the difficulty in controlling light and diverting its path on Silicon need to be addressed before this technology can be successfully used to resolve current microelectronics interconnect bottlenecks [2]. Investigation of solutions to the interconnect bottleneck has stimulated much research into actively controlling and manipulating the propagation of light through materials. Along this course of technological progress there has been much interest in the development of a photonic analogue to the electronic semiconductor. This requires the design and fabrication of photonic materials that can control and manipulate light on a microscopic scale [3]. This research has led to the development of photonic crystals (PhCs) or Photonic Band Gap (PBG) materials, structures which prohibit the propagation of certain wavelength ranges of light in certain directions depending on their physical properties.

1.1 Photonic Crystals

Since the invention of the laser, progress in Photonics has been intimately related to the development of optical materials which allows one to control the flow of electromagnetic radiation or to modify light matter interaction. Photonic Crystals are a novel class of the optical materials which elevates this principle to a new level of sophistication [1]. The PhCs are materials with a periodic modulation (translational symmetry) of the dielectric constant. This modulation gives rise to what is known as a Stop Band (SB), or a Photonic Band Gap within the crystal [4, 5]. The easiest way to understand the PBG effect is to rely on an analogy with natural crystals, which is a periodic repeated arrangement of atoms and molecules in space. A crystal therefore presents a periodic potential to electron propagation through it, and the geometry of the crystal dictates the energy band structure of the crystal, so that (due to Bragg-like diffraction from the atoms) electrons are forbidden to propagate with certain energies in the certain directions. For example, a semiconductor has a band gap between the valence and the conduction energy bands.

The PhCs are the artificial optical analogy of the natural crystals, in which the periodic “potential” is due to a lattice of microscopic dielectric media instead of atoms. If the dielectric constants of the materials in the crystal are different enough, and the absorption of light by the material is minimal, then scattering at the interfaces can
produce many of the same phenomena for the photons (light modes) as the atomic potential does for electrons [3].

The benefits of such a photonic band gap for direct-gap semiconductors are illustrated in Figure 1-1. On the right-hand side is a plot of the photon dispersion (frequency versus wavevector). On the left-hand side, sharing the same frequency axis is a plot of the electron dispersion, showing conduction and valence bands appropriate to a direct-gap semiconductor. Since atomic spacings are 100 times shorter than optical wavelengths, the electron wavevector must be divided by 1000 in order to fit on the same graph with the photon wavevector. The dots in the conduction and valence bands are meant to represent electrons and holes respectively.

If an electron were to recombine with a hole, they would produce a photon at the electronic band-edge energy. As illustrated in Figure 1-1, if a photonic band gap overlaps the electronic band edge, then the photon produced by electron-hole recombination would have no place to go [6].

![Figure 1-1](image)

*Figure 1-1: On the right is the electromagnetic dispersion, with a forbidden gap at the wavevector of the periodicity. On the left is the electron wave dispersion typical of a direct-gap semiconductor, the dots representing electrons and holes. Since the photonic band gap straddles the electronic band edge, electron-hole recombination into photons is inhibited. The photons propagation is prohibited [6].*

Depending on the number of directions that the SB (or PBG) exists in, there are one-dimensional, two-dimensional and three-dimensional photonic crystals (Figure 1-
2). If, for some wavelength range, a photonic crystal reflects light of any polarization incident at any angle, then the crystal has a complete photonic band gap (or omni-directional band gap). Only a 3D periodicity, with a more complex topology than is shown here, can support a complete photonic band gap. However, over the last decade, the focus of research groups has returned to 1D PhCs, due to their unique property to possess an omni-directional reflection, i.e. the presence of highly reflective bands over a wide range of angles of incidence and for both polarizations of light [7-9].

**Figure 1-2:** Simple examples of one-, two-, and three-dimensional photonic crystals. The different colors represent materials with different dielectric constants. The defining feature of a photonic crystal is the periodicity of material along one or more axes [3].

### 1.2 Si based Photonic Crystal devices

Recent advances in nano-, micro- and submicron-structuring technology provide an enormous flexibility in the choice of material composition, lattice periodicity and symmetry of the period arrangements allowing one to fabricate multi-dimensional PhCs operating in a wider range of electro-magnetic waves. For example, a PhC of a given geometry with millimeter dimensions can be constructed for control of microwave radiation, while with micron dimensions for control of infrared radiation. In this regard Silicon is the most attractive optical material from the variety of other different suitable materials mainly due to its transparency in the Near Infrared (NIR) range for both 1.3 and 1.55 μm telecommunication wavelengths as well as in the middle-infrared (MIR) and long-wave infrared ranges up to 100 μm. The success in the development of the in-plane light emitters and other microphotronics elements based on
monocrystalline Si, made the realization of all-Silicon optoelectronic circuits to be possible [10]. The term of "Silicon microphotonics" was first introduced by Lionel C. Kimerling in Ref. [11]. Briefly, the Si microphotonics is the optical equivalent of microelectronics for integrated circuits. It enables interconnection bandwidth that is not limited by the resistance, capacitance and reliability constraints of metal lines.

Modern Si fabrication technology allows fabrication of the PhC structures on nano-, micro-scale and of all dimensions on a single integrated platform. Examples of in-plane PhC realized on Si substrate are demonstrated in Figure 1-3.

Figure 1-3: SEM images of PhCs on Si platform: a) one-dimensional periodicity porous Silicon Bragg mirrors fabricated by vertical anisotropic etching of Silicon [12]; (b) two-dimensional hexagonal porous Si structure fabricated by anodization of p-type Silicon [12]; (c) three-dimensional Silicon photonic crystal woodpile structure fabricated by successive multiple masking-etching-alignment steps [13].
The Si-based photonic crystal structures have provided a good platform for numerous opto-electronic devices with applications in optical interconnects, chemical- and bio-sensing and etc. Below are some examples of utilization of 1D and 2D photonic crystals based on Silicon:

- **Photonic crystal waveguides**, obtained by realization of line defect within perfect periodical PhC structure [13]:
  - 2D-in-1D hybrid photonic crystal waveguide device fabricated by dry etching of Silicon (Figure 1-4) [18];

  ![Figure 1-4](image1)

  **Figure 1-4**: 2D-in-1D PhC waveguide for the measurements at 90° [18].

- Hollow waveguide with multilayer pairs of Si/SiO₂ coated on Si substrate (Figure 1-5) [19];

  ![Figure 1-5](image2)

  **Figure 1-5**: a) Schematic structure of hollow waveguide; b) SEM image of cross-section of hollow waveguide [19].
• **Photonic crystal fibres.** The total internal reflection phenomenon in photonic crystal fibres achieved by forming a two-dimensional photonic crystal around a hollow or Silica core [14, 15];

• **Photonic Crystal Microresonators,** realized by introduction of the defects/cavities within regular periodical structure [16, 17];
  
  - Microresonators based on nano-, meso-porous Si 1D photonic crystal with defects [20] (Figure 1-6);

![Figure 1-6:](image)

Figure 1-6: (a) SEM image of a Porous Silicon microcavity. (b) Resonance peak realized within the PBG at 0.63 nm [20].

• Microresonators based on macro-porous Silicon 2D photonic crystal with point defect [16] (Figure 1-7(a)) ;

• Microresonators based on photonic crystal waveguides with defect/cavities [21] (Figure 1-7(b));
Figure 1-7: A point defect (cavity) realized in (a) macro-porous Silicon photonic crystal [16] and (b) in photonic crystal waveguide fabricated by X-ray lithography [21].

- Microresonators based on grooved-Silicon 1D PhC, fabricated by means of e-beam lithography and dry etching of Silicon [22] (Figure 1-8);

Figure 1-8: (a) Optical image of the “fiber-photonic crystal-fiber” system; (b) Microresonators based on 1D PhC with defect; (c) Mirror based on 1D PhC [22].
1.3 Tunable Photonic Crystal Devices

One of the most important functions of the integrated Si-based photonic devices is the tuning capability of the optical characteristics by application of the electric field or by changing the temperature. The ability to modify the parameters of PBGs and resonances in a controllable way after PhC fabrication is a desirable property. The PBG parameters, e.g. bandwidth and wavelength of operation, depend on the structure of the crystal and on its constituent materials. The large variety of promising applications of photonic crystals depends on many adjustable parameters [1]. For the Si based PhCs the tuning of the optical properties can be achieved by either varying the optical thickness of Si/filler materials or by changing the geometrical parameters of the structure. If we can externally alter the materials and/or the structure during the device operation, we have an actively tunable PhC device (Figure 1-9). For example, in Si-based 1D and 2D PhCs the refractive index of Si can be altered by varying the temperature and the donor concentration, through the variations of the free carrier concentration [23].

In paper [24] the tuning of Silicon refractive index was experimentally demonstrated by injection of free carriers with 800 nm, 300 fs pulses, which allows ultra-fast band-edge tuning of 2D Si PhC. Also, the injection of free-carriers at any point of the p-i-n/cavity region can be used for the ultra-fast modulation of light in the waveguide [2]. Although, this method provides ultra-fast operation of the device (~1 ns), the associated relative spectral shift is very small, as the refractive index changes $|\Delta n|$ are below $10^{-3}$.

Alternatively, the refractive index of Silicon can be tuned by changing the temperature. In work [25] this effect was utilized in the optical filter based on 1D Si PhC fabricated by deep reactive ion etching. However, as for the previous tuning examples, the relative spectral shift is limited to the maximum variation of Si refractive index.

Microelectromechanical systems (MEMS) technology provides an attractive approach to provide the mechanical tuning mechanism, thus enabling a low-cost highly integrated tunable PhC filter. By varying the geometrical parameters of the PhC devices, e.g. filling fraction and size of the cavities, the precise position of the PBGs, band edges and/or resonances can be tuned or switched ON/OFF [1, 26-28]. The mechanical movement is controlled by either simple digital electronics or by means of the electrostatic deflection. However, current MEMS technology is capable of
producing mechanical devices that are on the scale of 10 to 500 μm [29], which limits the maximum tunability of the device.

**Methods of Active Tuning in Si Photonic Crystal devices**

![Diagram showing methods of active tuning in Si Photonic Crystal devices]

*Figure 1-9: Methods of active tuning (green) and correspondent parameters of tuning (blue) that can be realized in Si based Photonic Crystal devices.*

Significantly wider tunability can be achieved for the non-mechanical design of composite PhC devices, based on Silicon and various filler-materials that can change their optical characteristics by changing temperature or applying the electric field. In this regard, the most promising filler-material is considered to be liquid crystal (LC) with its extraordinary optical properties. Firstly, LCs show large optical birefringence in which molecular reorientations can be induced by low power electric fields. Secondly, the LCs possesses high transparency, low absorption and scattering losses in a wide wavelength range span from visible to middle infrared. One of the disadvantages of the existing up to date commercial nematic LC, suitable for this purpose, is a slow response time. However, recently the MEMS-driven tuning of the liquid crystal fillers was demonstrated providing much shorter response time than using temperature and electric field [30]. A brief introduction and background of tunable LC-infiltrated photonic crystals are reviewed in the following Section.
1.4 Photonic Crystals and their liquid crystal composites

Liquid crystals combine fluid behaviour and anisotropic properties in a unique way. Anisotropy, i.e. the dependence of bulk material properties on the crystallographic direction, indicates non-spherical symmetry of the corresponding material. This phenomenon is traditionally attributed to solid crystals. However, organic compounds that consist of molecules with anisotropy of shape (for example rod-like or disk-like) can show an orientational order of these molecules even in a fluid state. If so, this fluid state is referred to as being the liquid crystalline state. Thermotropic, calamatic LCs consist of rod-like organic molecules which form mesophases. These mesophases exist between the conventional crystalline phase and the isotropic liquid phase (Figure 1-10).

The most common LC mesophase is the nematic which is characterized by uniaxial orientational order, i.e. one preferred axis is sufficient to describe its local anisotropy. The director \( \mathbf{N} \) (a pseudo vector) can be used to indicate the local molecular alignment and a scalar order parameter \( S \) is sufficient to describe the degree of orientational order [1, 31].

![Diagram of phase transition](image)

**Figure 1-10:** The nematic liquid crystal mesophase has an orientational order, but lacks of a long-range positional order, and exists between the crystalline and isotropic phases. \( \mathbf{N} \) is the nematic director [32].

The most important anisotropic property from the optical point of view is birefringence. The effective refractive index for linear polarized light with the direction of the electric field vector perpendicular to the director (ordinary refractive index \( n_o \)) is
different from the effective value for polarized light with the direction of electric field vector parallel to the director (extraordinary refractive index \( n_e \)). The difference between these two effective refractive indexes is called birefringence of LC, \( \Delta n_{le} = n_e - n_o \), and can be as large as 0.3. The birefringence of thermotropic LC \( \Delta n_{lc} = n_e - n_o \) decreases with increasing temperature (decreasing orientational order) and vanishes above the nematic-isotropic transition temperature (clearing temperature for nematic LC).

There are numerous publications devoted to experimental investigations of the electro-tuning effect in LC photonic structures such as LC-opal composite structures [33-35], micro-porous “Si-LC” structures [36, 37] and multilayered 1D PhC with liquid crystal cavity [38] which manipulate with light propagating perpendicular to the substrate. The number of papers dealing with the molding of in-plane light propagation is relatively small and these mainly present the results on the thermo-tuning effect in 1D and 2D PhCs. One of the main reasons for that is the difficulty with the application of an electric field to the matrices based on electro-conductive materials. Also, the response time for the nematic LC is in the range of milliseconds, which makes the LC material not very suitable for optical interconnect applications.

However, today, “Si-LC” based photonic research is undergoing a modern-day renaissance. For example, bio-sensors fabricated with LC and Si materials can allow label-free observations of biological phenomena. Moreover, as it will be demonstrated in Chapter 4, the continuous electro-tunability of LC filler in the optical devices based on PhC may be used for compensation of the post-fabrication tolerances and, thus, adjustment of the optical device to its nominal operational mode.

1.5 Thesis Overview

Chapter 1: An introduction to Photonic Crystals and their application in integrated Silicon photonics is presented. The contexts in which this body of work was performed and the motivation behind the studies contained therein are outlined.

Chapter 2: The basic concepts of theoretical and experimental background are introduced. A classic model of 1D PhC is described for the grooved Silicon case. The methods used for fabrication of the grooved Silicon structures in this work are
discussed. The optical experimental techniques applied to the investigation of the fabricated structures are described.

Chapter 3: In this Chapter, the design of a new type of 1D Si PhC based on multi-component model is described. The fabrication techniques for realization of multi-component PhCs by introduction of additional regular layers into a grooved Silicon structure are discussed. The novel optical effects such as omni-directional PBGs and ultra-wide regions of transparency have been obtained for the suggested model. Based on the obtained results the band-pass filter based on three-component PhC structure was fabricated and successfully examined experimentally in Mid-IR.

Chapter 4: The model of transformation of defect-free photonic crystal structures into tunable Fabry-Perot resonators on Si chip is theoretically described and experimentally demonstrated. The transformation is achieved by introduction of the optical defects into certain periods of grooved Silicon structures. The ultra-wide and electro-controllable tunability is experimentally demonstrated for the Fabry-Perot filters based on Si and nematic liquid crystal. Furthermore, a technique for precise position control of individual transmission resonances/channels in a triple Fabry-Perot filter is also proposed.

Chapter 5: An approach for investigation of the photonic band gap deviations caused by structural fluctuations in fabricated one-dimensional photonic crystals is demonstrated. The deviations of the photonic band gaps are strongly dependant on the magnitude of the structural fluctuations and demonstrate an increase with the order of the photonic band gaps. The approach is proposed for the determination of the fabrication tolerances and optimization of the photonic band gap properties of the fabricated photonics crystal structures.

Chapter 6: Finally conclusions and future work are drawn.
1.6 References


Chapter 2.

Theoretical and Experimental Background

2.1 Introduction

In this Chapter, the basic concepts of the simulation, and experimental fabrication and characterization techniques employed to study the optical properties of the in-plane grooved Silicon photonic crystal structures are discussed. The design of one-dimensional photonic crystals and the analysis of their optical properties have been performed using transfer matrix [1] and forbidden gap map (GM) methods [2]. The GM method is one of the most powerful design methods since it can be applied to modelling of PhCs with any possible geometrical configurations, e.g. PhCs with defects [3], disordered PhCs [4], multi-component PhCs [5] and others, providing the optimal design parameters using a single graphical representation. For the fabrication of grooved Silicon structures two etching techniques were employed: Wet Anisotropic Etching (WAE) of (110)Si in an aqueous solution of potassium hydroxide (KOH) and Deep Reactive Ion Etching (DRIE) of (100)Si. WAE produces good quality smooth mirror like side-walls which is important for obtaining PBGs with high reflection. However, WAE can only be performed on (110)Si. DRIE can be performed on (100)Si and hence it is compatible with current processing technology. The optical characterization of the photonic properties of fabricated structures was mainly performed using the Fourier Transform Infrared (FTIR) microspectroscopy in mid-IR range and using optical-fiber-coupling set-up based on an optical spectrum analyzer (OSA) in near-IR range.
2.2 Calculation methods

2.2.1 The Transfer Matrix Method

The transfer matrix method is a 2x2 linear matrix describing light propagation in a stratified medium. A stratified medium is a medium whose properties are constant throughout each plane perpendicular to a fixed direction. The TMM is based on the fact that the equations that govern the propagation of light are linear and the continuity of the tangential fields across an interface between two isotropic media can be regarded as a 2x2 linear-matrix transformation [1, 6]. One of the most attractive features of the TMM method is the ease of introducing any number of different additional layers (strata) and defects at any point in the TMM’s matrix equation, which enables the engineering of various complicated 1D PhC devices for different applications [7, 8].

Consider a stratified structure that consists of a stack of 1, 2, 3,...,j,...,N parallel layers (strata) placed in (0) media (Figure 2-1). Let all media be linear homogeneous and isotropic, and let the complex index of refraction of the j-th layer be \( n_j \) and its thickness \( d_j \). The complex index of refraction of (0) media is \( n_0 \).

Figure 2-1: Reflection, \( R \), and transmission, \( T \), of a plane wave by a multi-layer structure with high and low refractive indexes of layers. \( \theta \) is the angle of incidence.

An incident monochromatic plane wave in medium (0) generates a resultant reflected plane wave, \( R \), and a resultant transmitted plane wave, \( T \). The total field inside the j-th layer, which is excited by the incident plane wave, consists of two plane waves: a forward-travelling plane wave denoted by (+), and a backward travelling plane wave denoted by (-).
The wave-vectors of all plane waves lie in the same plane (the plane of
incidence), and the wave-vectors of the two plane waves in the j-th layer make equal
angles with the z-axis which is perpendicular to the plane boundaries. When the incident
wave in the ambient is linearly polarized with its electric vector vibrating parallel (TE
or E) or perpendicular (TM or H) to the plane of incidence, all plane waves excited by
that incident wave in the various layers of the stratified structure will be similarly
polarized, parallel or perpendicular to the plane of incidence, respectively. In the
following, it will be assumed that all waves are either TE(E)- polarized or TM(H)-
polarized.

Let $E^+(z)$ and $E(z)$ denote the complex amplitudes of the forward- and
backward-travelling plane waves at an arbitrary plane z. The total field at z can be
described by a 2x1-column vector.

$$E(z) = \begin{bmatrix} E^+(z) \\ E^-(z) \end{bmatrix} \quad (2.1).$$

If we consider the fields at two different planes $z'$ and $z''$ parallel to the layer boundaries
then, by virtue of system linearity, $E(z'')$ and $E(z')$ must be related by a 2x2 matrix
transformation

$$\begin{bmatrix} E^+(z') \\ E^-(z') \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} E^+(z'') \\ E^-(z'') \end{bmatrix} \quad (2.2).$$

More concisely, Eq. (2) can be written as

$$E(z') = SE(z'') \quad (2.3),$$

where

$$S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \quad (2.4).$$

Note that S must characterize that part of the stratified structure confined between the
two parallel planes at $z'$ and $z''$. By choosing $z'$ and $z''$ to be immediately adjacent to the
0-1 and N-0, interfaces respectively, Eq. (2.3) will read

$$E(z_1 - 0) = SE(z_0 + 0) \quad (2.5),$$
where \( z_I \) and \( z_0 \) are adjacent media to the 01 interface.

Equation (2.5) defines a scattering matrix, \( S \), which represents the overall reflection and transmission properties of the stratified structure. \( S \) can be expressed as a product of the interface and layer matrices, \( I \) and \( M \), that describe the effect of the individual interfaces and layers of the entire stratified structure, taken in proper order, as follows:

\[
S = I_{01} M_1 I_{12} M_2 \ldots I_{(j-1)j} M_j \ldots M_N I_{NO} \quad (2.6).
\]

The matrix \( I_j \) of an interface between two adjacent layers \( j-1 \) and \( j \) (7), and the matrix \( M_j \) of the layer \( j \) (2.8):

\[
I_j = \begin{bmatrix}
1 & r_j \\
1 & t_j
\end{bmatrix} \quad (2.7)
\]

\[
M_j = \begin{bmatrix}
e^{i\beta_j} & 0 \\
0 & e^{-i\beta_j}
\end{bmatrix} \quad (2.8),
\]

where \( r_j \) and \( t_j \) are the interface Fresnel coefficients of reflection and transmission, respectively, and the phase shift (phase thickness of the layer), \( \beta \), is given by (2.9):

\[
\beta_j = 2\pi \left( \frac{d_j}{\lambda} \right) n_j \cos \theta \quad (2.9),
\]

where \( \lambda \) - wavelength; \( n_j \) - refractive index of \( j \)-th layer, \( d_j \) - thickness of \( j \)-layer and \( \theta \) - angle of incidence.

From the matrices of interface, \( I \), and layer, \( M \), the overall scattering matrix \( S \) of the stratified structure can be found by straightforward matrix multiplication:

\[
\begin{bmatrix}
E_0^+ \\
E_0^-
\end{bmatrix} = \begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix} \begin{bmatrix}
E_0^+ \\
0
\end{bmatrix} \quad (2.10),
\]

where, for simplicity, the subscripts 0 and \( \theta_S \) refer to the semi-infinite air input and output media, respectively, and \( E_{0_S}^- = 0 \). Further expansion yields the total reflection, \( R \), and transmission, \( T \), coefficients of the stratified structures as

\[
R = \frac{E_0^-}{E_0^+} = \frac{S_{21}}{S_{11}} \quad (2.11),
\]

\[
T = \frac{E_0^+}{E_0^+} = \frac{1}{S_{11}} \quad (2.12),
\]

respectively.
2.2.2 Modelling of grooved Si structures

In this work, a One-Dimensional Photonic Crystal structure was investigated by modeling it as a free-space microstructured grooved Silicon structure with linear grooves, as shown in Figure 2-2. The refractive index of Si for the high-refractive index layer, \( n_H = n_{Si} = 3.42 \), in the mid- and near-IR range, is considered in accordance with Reference [9]. Since the modelling was performed for normalized frequency (wavelength) range, which allows to design of PhC structure for operation in a wide IR range, the dispersion of Si was not taken into account. The structure is operating in the free space; therefore the refractive index of the incoming and outgoing medium is 1. A considerable advantage of these 1D PhCs is that the air grooves (the low-refractive index layer, \( L \)) with refractive index \( n_L = n_{air} = 1 \), can be easily infiltrated with filler whose refractive index is different from air. In the case of the original “Si-air” structure, the optical contrast is \( n_H/n_L = n_{Si}/n_{air} = 3.42/1 \) and the structure can be considered as a high-contrast PhC. Therefore, only a small number of periods is needed in order to obtain a PBG with a reflectance, \( R \), of over 99% and a substantial edge sharpness. The optical spectra of this structure can be calculated using the TMM.

![Figure 2-2: Schematic fragment of grooved-Si structure with (a) air grooves and (b) grooves infiltrated with LC.](image)

As all thicknesses of periods are the same for this type of grooved Silicon structure, the equation (2.6) can be written in more compact form:

\[
S = [(I \cdot M)_{Si} \cdot (I \cdot M)_{air}]^N \cdot (I \cdot M)_{Si} \tag{2.13},
\]
where \((I\cdot M)_\text{Si}\) and \((I\cdot M)_\text{air}\) are the optical matrixes of the Si and air layers, \(N\) is the number of periods in the structure, \(I\) is the matrix of the interface between the layers and \(M\) is the matrix of the layer transmission.

The value \(I\) depends on the refractive indexes of the components of the periodic structure, while the value of \(M\) depends on their thickness, \(d\), and on the wavelength, \(\lambda\). In accordance to the Eq. (2.11-12), the reflection coefficient, \(R(\lambda)\), and the transmission coefficient, \(T(\lambda)\), can be calculated from the following equations

\[
R(\lambda) = \left[ \frac{S(\lambda)_{11}}{S(\lambda)_{21}} \right]^2 \quad (2.14),
\]

\[
T(\lambda) = \left[ \frac{1}{S(\lambda)_{11}} \right]^2 \quad (2.15),
\]

respectively.

### 2.2.3 Design of the Photonic Band Gap characteristics

The design of grooved Si structure with desired photonic band gap characteristics normally starts with the selection of the wavelength \(\lambda\) of its operation. Then, the materials with corresponding refractive indexes, \(n_L\) and \(n_H=n_{Si}\), for suitable periodic structure fabrication are chosen. Based on the above selection, the geometrical thickness of both components, \(d_L\) and \(d_{Si}\), are determined in accordance with the Bragg condition

\[
\frac{\lambda}{2} = n_{Si} \cdot d_{Si} + n_L \cdot d_L \quad (2.15),
\]

where \(n\cdot d\) is the optical thickness of the corresponding high-(H) and low (L)-refractive index components. For equal optical thicknesses of each component \(n\cdot d=\lambda/4\), the maximum width of the PBG (or stop-band (SB)) is achieved for the required wavelength \(\lambda\).

The PBG properties of the grooved Silicon structure are strongly dependent from the following design parameters:

- Optical contrast of layers, \((n_{Si}/n_L)\)
- Lattice constant, \(a=d_{Si}+d_L\) (Figure 2-2)
- Filling fraction of Si, \(f_{Si}=d_{Si}/a\)
• Number of periods, $N$.

A precise control of these parameters over the design and fabrication process is obviously necessary for the proper operation of the PhC device. The value of lattice constant, $a$, is normally very well controlled during the fabrication process and, so, by varying only thickness of Si, $f_{Si}=d_{Si}/a$ and/or the refractive index of the $L$-layer, $n_L$, the following general PBG parameters can be altered:

• order of PBGs;

• wavelength of operation of PBGs;

• width of the PBGs;

• vanishing and splitting of the PBGs.

2.2.4 Gap Map Approach

The design procedure requires the investigation of the influence of all nominal parameters listed above on optical characteristics of PhC devices, this makes the design part very complex involving calculation and analyses of the vast number of spectra. Several approaches can be used in order to determine the optical properties of a 1D PhC. One of these is to calculate the band diagrams (BD) [10] for the selected filling fractions $f_{Si}=d_{Si}/a$. The second design approach is based on the Gap Map (GM) presentation, which was first suggested by John D. Joannopoulos et al. in Ref. [2]. For drawing the GM, in principle, both the BD [11] and the reflection spectra calculation method [1] can be used. The calculation of the reflection spectra of 1D PhC with the certain number of lattice periods is normally performed using the TMM [12]. The GM approach is one of the most attractive design tools for the band-gap structures [11, 13] as well as tunable [12] and composite [14] photonic structures, since it allows quick and easy analysis of structures for a large set of spectra (normally over 100) to be done practically on one plot.

Using the transfer matrix method, the set of reflection spectra, $R$, for sequential values of filling factor, $f_{Si}$, in the range from 0 and 1 is calculated. For each of the calculated spectra, the values of $\lambda$ (or wavenumber, $\nu$) for which $R>99\%$ (PBG regions), are plotted against $f_{Si}$ as shown in Figure 2-3(a). For the structures with smaller number of periods, e.g. elementary Fabry-Perot unit with $N=1.5$, this level was lowered to $R>85\%$ for more clear representation, as in this case the map represents the
regions of high reflectivity (SBs). The PBG GM allows an effective comparison of PhC structures with various number of periods, \( N \), lattice constant, \( a \), refractive index contrast, \( \Delta n = n_{Si}/n_{L} \), angle of incidence, \( \theta \), and polarization of the incident light.

An example of the reflection spectrum which constitutes the Gap Map is shown in Figure 2-3 (b). As lattice constant, \( a \), is kept constant, prediction of the wavelength range in which a PhC with a particular \( d_{Si} \) will operate is possible. Alternatively, the \( d_{Si} \) which is necessary to obtain a PhC over a certain wavelength range can be determined. For example, it can be determined from Figure 2-3(a) that the wavelength range of the main PBG of a PhC with the parameters \( f_{Si}=0.226 \) and \( a=4 \) \( \mu \)m is between \( \lambda=10 \) \( \mu \)m and \( \lambda=15.5 \) \( \mu \)m. Alternatively, if required criteria is to design a PhC with a PBG with a maximum width between \( \lambda = 14 \) \( \mu \)m and \( \lambda = 20 \) \( \mu \)m, the optimal design parameter would be \( f_{Si} = 0.6 \) for the main PBG.

\[ \Delta f_{Si} \]

**Figure 2-3:** (a) Calculations of the main PBG (1) and secondary PBGs (2, 3 etc.) for a 1D PhC based on the grooved Si with number of periods \( N=50 \), \( a=4 \) \( \mu \)m at normal incidence of light. (b) Calculated reflectance spectrum of the structure with \( f_{Si}=0.226 \).

Using Figure 2-3(a) it is also possible to determine the maximum fabrication tolerances of the designed structure. The range of filling fraction \( \Delta f_{Si} \) for which the main
PBG characteristics, such as bandwidth, operational wavelength and flat-top 100% reflection, remain the same, can represent the maximum lithography error for the fabrication of the grooved Si structure. Obviously, as it can be seen in Figure 2-3, the high order PBGs demonstrate the highest lithography tolerances (the PBG regions are located almost parallel the filling fraction axis) comparing to the lowest PBGs. For example, the PhC mirror with $f_{Si}=0.6$ and operating at the 3rd PBG and reflecting light from 5.00µm to 5.75µm has the fabrication tolerance $\Delta f_{Si}=0.05$, which is 200 nm for the considered example with $a=4$ µm.

By using the normalized ranges of frequencies, $NF=a/\lambda$, or normalized wavelengths $NW=\lambda/a$, the Gap Map becomes universal and therefore can be applied to a wide range of structure sizes including micro- and nano-structures.

2.3 Fabrication methods

Modern micromachining of semiconductors allows the construction of PhCs with high optical contrast and high dimensional tolerances. A preliminary templating of a Si wafer with subsequent electrochemical or chemical etching through the template is used for the initial patterning. A template is usually produced by means of lithography. The classical optical lithography offers the possibility of fabrication of patterns with the minimum size of ~1 µm.

In general, there are two classes of etching processes:

1. Wet etching, where the material is dissolved when immersed in a chemical solution

2. Dry etching where the material is sputtered or dissolved using reactive ions or a vapour phase etchant

In the following Sections, we will briefly discuss Wet Anisotropic Etching and Deep Reactive Ion Etching techniques that were used in this work.

2.3.1 Crystallographic Orientation of Silicon

A crystal is a solid in which the constituent atoms, molecules, or ions are packed in a regularly ordered repeating pattern extending in all three spatial dimensions. Atoms in a crystal arrange themselves at specific points in a structure known as a unit cell. The unit cell structure is repeated everywhere in the crystal [15]. In single crystal
materials the unit cells are all neatly and regularly arranged to each other while in polycrystalline crystals they are not. Silicon wafers are single crystalline materials.

Crystalline materials have two main features which affect most of their properties, namely anisotropy and symmetry. Crystal anisotropy arises from the fact that interatomic distances and forces vary in different directions and are regular at the same time. Hence, the properties of the crystal vary in different directions but are the same in parallel directions. The symmetry of crystals is due to the symmetry of the crystal lattice. The symmetry of a single crystal arises from the repeating symmetry of its lattice.

Crystal planes in single crystal are identified by a series of three numbers known as the Miller indexes. This theory can be conceptualised as slicing a single crystalline block at different angle to expose different planes with different properties. The (100), (110) and (111) planes defined by the Miller indexes are shown in Figure 2-4. Miller indexes characterise all planes parallel to the plane concerned. The two most common orientations used for Silicon wafers are (100) and (111) planes [15].

![Figure 2-4: Planes defined by the Miller indexes.](image)

### 2.3.2 The Wet Anisotropic Etching Technique of (110) Si

This wet etching is the simplest etching technology. There are actually two types of wet etching: isotropic and anisotropic etching (Figure 2-5). Wet isotropic etching is a uniform etching process that decays in the Si material at the same rate in both vertical and horizontal directions while anisotropic etching decays in the material in a more selective direction (Figure 2-5). For wet anisotropic etching of Silicon the
aqueous solution of KOH with addition of alcohols and a number of other anisotropic etchant is typically used [16]. In 1979, Kendall reported the fabrication of extremely narrow grooves in Silicon due to this technique and forecast that this would probably spawn a number of technological revolutions [17]. However, the technique is not widely used in the fabrication of optical elements, despite the possibility of fabricating periodic structures with high refractive index contrast and smooth mirror-like side-walls in Silicon transparency range [18].

![Figure 2-5: Difference between (a, b) anisotropic and (c) isotropic wet etching [19].](image)

Fabrication of grooved Si by the wet anisotropic etching of (110) Silicon in KOH is based on the difference in the etching rate for the (110) and (111) crystallographic planes [20]. The main etching rules of mono-crystalline Si of different crystallographic orientations were established in seventies of the last century [21] and can be summarized as:

i) The ratio of the etching rates is highly dependent on the crystallographic orientation. The ratios of the etch rate for the (111), (110) and (100) planes in 44% KOH at 70°C are related as $V_{111}:V_{110}:V_{100} = 1:600:300$ [17]. Therefore, this technique is only compatible with (110) Silicon.

ii) The etch rates of SiO$_2$ or Si$_3$N$_4$ in KOH solution are hundreds of times smaller than the etch rate of Silicon. This enables their use as a protective mask for forming patterns using relevant methods of lithography and to etch through these patterns the air holes of different shape.
For this work, (110)-oriented Si is of a principal interest. If long, narrow windows, precisely oriented along the (111) plane trace, are patterned in the masking film via lithography, the trench walls obtained in the Silicon after anisotropic etch are oriented perpendicular to the substrate plane. The method permits the fabrication of deep trenches of various widths with smooth side-walls of optical quality without under-etch of the sidewalls (Figure 2-6). As it was demonstrated in the past [20], this technology could be used for the fabrication of 1D PhCs for in-plane infrared light propagation.

Figure 2-6: (a) SEM image of Si walls for periodic photonic structure, obtained by deep anisotropic etching of (110) Si. (b) The optical microscopy image of 1D PhC, fabricated by WAE method: the top view of structure with lattice period \(a=7\mu m\).

The WAE method is also suitable for fabrication of defects in the periodic structure, which can be used as micro-cavities. Using the WAE method allows PBG structures to be fabricated on an SOI substrate. This offers advantages in receiving the total internal reflection in planar waveguides and provides electrical isolation from the substrate. The latter is crucial in the fabrication of electro-tunable PBG devices, as will be shown in Chapter 4. However, WAE methods have also some disadvantages. (110)-oriented Si substrates are expensive and not in use in mass-production. In addition, it is imperative to precisely align the lithographic mask with the Silicon crystallographic axes, increasing the difficulty of the technique. Cross cut walls of the trenches are tilted and this results in an ineffective use of the substrate area. The long side of the grooves can be only oriented along two directions in the (110) plane which form the angle of 70.50°. This places substantial restrictions on the structure design, and may result in
undercutting where elements cross. DRIE etching of Si does not suffer from these disadvantages.

2.3.3 The Deep Reactive Ion Etching Technique of (100) Si

Dry etching is a generic term that refers to the etching techniques in which gases are the primary etch medium, and the wafers are etched without wet chemicals and rinsing. The wafers enter and exit the system in a dry state. The dry etching technology can split in three separate classes called reactive ion etching (RIE), plasma, and ion beam milling (etching) [15].

In RIE, the Silicon wafer is placed inside a reactor in which several gases are introduced. Plasma is struck in the gas mixture using a radiofrequency (RF) power source, breaking the gas molecules into ions. The ions are accelerated towards, and react at, the surface of the Si material being etched, forming another gaseous material. This is known as the chemical part of reactive ion etching. There is also a physical part which is similar in nature to the sputtering deposition process. If the ions have high enough energy, they can knock atoms out of the material to be etched without a chemical reaction. It is a very complex task to develop dry etch processes that balance chemical and physical etching, since there are many parameters to adjust. By changing the balance it is possible to influence the anisotropy of the etching, since the chemical part is isotropic and the physical part highly anisotropic the combination can form sidewalls that have shapes from rounded to vertical. A schematic of a typical reactive ion etching system is shown in Figure 2-7.

A special subclass of RIE which was used for fabrication of the PhC structures in this work is deep RIE (DRIE). DRIE systems combine plasma etching and ion etching principles [22]. DRIE is a combination of three primary processes, etching, passivation and ion bombardment. A highly reactive gas is used to perform an isotropic etch of the substrate. After a brief period the etching is stopped and a passivation layer is deposited over the whole surface of the substrate. This protects the substrate from chemical attack and prevents further etching. The process then returns to etching and a collimated stream of directional ions bombard the substrate. These ions remove the passivation layer from the bottom of the previous etch step, but not from the sides, in a process called sputtering. The etchant chemicals can then erode only the bottom of the channels. The process is repeated many times over resulting in a large number of very
small isotropic etch steps taking place only at the bottom of the etched pits. It is this selectivity that leads to the overall anisotropy of the process and the creation of high aspect ratio channels with vertical sidewalls. As a result, etching aspect ratios of 50 to 1 can be achieved. The process can easily be used to etch completely through a Silicon substrate, and etch rates are 3-4 times higher than wet etching.

**Figure 2-7:** Typical parallel-plate reactive ion etching system.

In Silicon micromachining a profile control of high-aspect ratio trenches (HARTs) is increasingly important. The aspect ratio is defined as the maximum depth divided by the maximum width. The HARTs give rise to the following specific problems:

- The aspect ratio dependent etching (ARDE) effects (Figure 2-8(a)):
  - RIE lag is associated to the effect that smaller trenches are etched at a different speed than wider trenches. It is explained in considering the depletion of reactive particles during their trajectory in the trench.
  - Bowing is the observation of a parabolic curvature of etched sidewalls as found for the wider opening.
  - Trench area dependent tapering of profiles is the effect that wider trenches have different slopes/tapering with respect to the smaller trenches.
• Bottling shows up as bottle-shaped trenches and is caused by ion shadowing and sharpening of the collimated ion beam incoming from the glow zone. Generally it is pronounced only at a high pressure (Figure 2-8(b)).

• Micrograss is the existence of long-tailed spikes at the trench bottom. Generally, the appearance of such rough surface is grey or even black (Figure 2-8(c)).

• Tilting is observed near geometrical obstacles and is due to boundary distortion or local differences in radical density. In the demonstrated Figure 2-8(d), the wafer edge is responsible for the tilting [23].

![Figure 2-8: SEM images of the grooved-Si structures fabricated by DRIE: (a) The ARDE effect, (b) Bottling of the grooves, (c) Micrograss in the grooves, (d) Tilting of grooves [21].](image)

Another disadvantage of DRIE method is the high interface roughness of the structures etched on the great depth (>10-15 μm), which results in the scattering losses of the light during the optical operation. In order to overcome these problems the DRIE etching technological process should be carefully controlled during the etching process. The DRIE process settings, the equipment parameters, the plasma characteristics, and the trench-forming mechanisms are responsible for the final HART profile and, therefore, should be carefully monitored during the etching process. Dry etching is one
of the most enabling technologies, which comes at a sometimes high cost. However, it remains the most preferable etching technique for fabrication of deep patterns with vertical side-walls, since it can be performed on all crystallographic orientations of wafer. Therefore, it is highly compatible with current CMOS processing.

Grooved Si samples were fabricated by this technique in Tyndall Institute Ireland, Cork, thanks to NAP94 (Prof. Tatiana Perova) and NAP368 (Anna Baldycheva, Prof. Tatiana Perova).

2.4 Methods of characterization

2.4.1 FTIR Microspectroscopy Technique

Fourier Transform Infrared Spectroscopy is a workhorse of the industrial materials testing division. The combination of a microscope with an infrared spectrometer results in a powerful instrument that allows analysis of very small photonic samples in a wide IR range. Indeed, infrared microspectroscopy has become the technique of choice for samples smaller than 100 μm, or where spectra of small areas within a large sample, like layers in a laminate or defects in a matrix, are required. Also, information about the chemical makeup, heterogeneity, and layers within the sample can be derived with infrared microspectroscopy.

The basic process in FTIR spectroscopy is light wave interference. The main component of a Fourier Transform Infrared spectrometer is the Michelson interferometer. The Michelson interferometer contains a fixed mirror, a movable mirror and a beamsplitter. The beamsplitter transmits half of the incident radiation to the moving mirror and reflects the other half to the fixed mirror. The two beams are reflected by these mirrors back to the beamsplitter, where they recombine. When the fixed mirror and the moving mirror are equidistant from the beamsplitter, the amplitudes of all frequencies are in phase and interfere constructively. As the moving mirror is moved away from the beamsplitter, an optical path difference is generated. A pattern of constructive and destructive interferences (interferogram) is generated depending on the position of the moving mirror and on the frequency of the radiation. This beam is then directed through the sample compartment to the broadband detector and a digital signal processor sorts out the signal corresponding to each frequency using a fast Fourier Transform (Figure 2-9) [24].
The Bio-Rad Digilab FTS 6000 spectrometer was used to measure reflection and transmission spectra in the wide range of 700-7000 cm\(^{-1}\) of photonic crystals structures. It consists of a step scan interferometer bench (FTS 6000) coupled to a MCT (HgCdTe) detector equipped with a microscope, UMA-500, for delivering a focused incident beam on the sample. One of the advantages of this particular system for reflection and transmission measurements on grooved Silicon is the possibility to form a rectangular shape of the incident beam on the sample using microscope aperture for increasing the signal-to-noise ratio. This setup allows the measurement of Si structure with a minimal incident beam aperture 10x10 \(\mu m^2\).

**Figure 2-9: Layout of a simple FTIR spectrometer.**

IR measurements of grooved Si are very critical to the direction of the light propagation through the whole structure. The IR beam should be exactly perpendicular to the Si walls along the entire path. For this reason a special sample holder, shown in Figure 2-10, has been used for the measurements. This allows adjusting the sample in the \(X-Y-Z\) direction.
Figure 2-10: (a, b) Schematic of the experimental set-up with IR beam focused by microscope on the grooved Si (position 1) and on bare Silicon (position 2). (c) Reflection characterization setup using a Fourier-transform infrared spectrometer coupled to an achromatic infrared microscope [25].

Certain difficulties arose during the measurements due to complicated structure of the samples. In particular, the part of the unetched Si walls at the bottom of the grooves masked both the incident and reflected IR beams, which reduced the intensity of the signal reaching the microscope objective. In order to avoid this “shading effect” from the Si substrate, which interfere with the cone of incident light, the photonic crystal structures were fabricated close to the edge of the substrate (Figure 2-10(b)). An infrared spectrum is generally displayed as a plot of the energy of the infrared radiation (expressed either in microns or wavenumbers) versus the percent of light reflected/transmitted by the sample. The reflection/transmission coefficients are obtained by dividing the spectra obtained with the PhC structure by the background.
spectra. The Single Beam reflection signal from the gold-coated glass ($R=0.99$) has been used as a reflection background, while Single Beam transmission signal without sample ($T=0.99$) has been used as a transmission background. Reflection of the bare crystalline Si was used for the comparison. For polarized FTIR measurements, the polarizer was placed before the microscope detector (Figure 2-10(c)).

2.4.2 End-fire Technique

For analysis of the structures in the near-infrared range (1200-1700 nm) an optical fibre-coupling set-up based on Optical Spectrum Analyser has been used. The free-space end-fire setup was mainly developed for the purpose of polarized transmission measurements of LC PhC resonators around the telecommunication wavelength range.

The coupling of light into guided modes by transverse excitation is known as the end-fire coupling method. End-coupling experiments involve the coupling of light into waveguide samples or free-space photonic samples that are end-polished with an optically smooth finish. End-fire coupling can be achieved by means of microscope objective lens focused on the sample or butt-coupling an optical fiber to the sample ends. In this work the free-space coupling was used to couple the light source into PhC structures. The schematic of the experimental setup is shown in Figure 2-11.

![Figure 2-11: Schematic of the setup for end-fire light coupling using microscope objectives (also known as free-space coupling).](image)

35
A broadband light source Oriel® Arc 75W Xenon Lamp that provides light with a broad wavelength range in the near infrared region from 1200 to 1700 nm was used. A light beam from a source was transmitted from the end of a single-mode fiber, through the polarizer and then focused on the sample using the microscope objective. The experimental setup typically comprises of trio of optical stages. The input and output components (i.e. microscope objectives) and the sample are separately mounted on high precision micro-positioners and micro-manipulators to achieve accurate and stable alignment. Transmitted light is then collected by the microscope objective and coupled to the single mode fiber which is connected to the optical spectrum analyzer Agilent 861408B, allowing the monitoring of the PBGs and resonance peaks. The measured transmittance is normalized by the light intensity measured without sample. Finally, the
results of these measurements are compared with theoretical calculations and FTIR measurements.

The TMM calculation method described in Section 2.2 considered for the parallel incident light beam for simulations of the optical spectra of photonic crystals. However, in both experimental techniques the incident light beam was focused with the maximal angle of the light cone up to 30°. The cone-shape of the light beam causes the degradation of the main PBG characteristics, e.g. smoothing of “Π”-shape, narrowing, shift and even disappearance of high-order PBGs [26].

2.5 Summary

The basic concepts of theoretical and experimental background have been introduced. A one-dimensional photonic crystal structure was investigated by modeling it as a free-space microstructured grooved Silicon structure with linear grooves. The utilization of the transfer matrix and forbidden gap map methods allows easier modelling of the optical properties of the grooved Silicon photonic crystals with additional components for realization of multicomponent photonic crystals (Chapter 3) cavities/defects for realization of the micro-cavity photonic crystals (Chapter 4) and disorder in geometrical parameters (Chapter 5). The introduction to the methods of Silicon microstructuring used for the fabrication of the grooved Silicon structures in this work has been discussed. The optical experimental techniques applied to the investigation of the fabricated multi-component photonic crystal and microcavity photonic crystal structures in a wide infrared range have been described.

2.6 References


Chapter 3.

Multi-Component Photonic Crystals

3.1 Introduction

The precise and technologically controllable engineering of the photonic crystal structures with optimal parameters is still remaining an art, requiring intuition as well as analytical knowledge to create a structure with unique properties. Indeed, these structures operate by the Photonic Band Gap effect and, therefore, possess high sensitivity to the refractive index, $n$, (or optical thickness) of their components. The PhCs are normally composed of two-components, with high ($n_{hi}$) and low ($n_{li}$) refractive indexes. By changing the value of $n_{hi}$ or $n_{li}$, tuning of the PBG position can be achieved.

As discussed in Chapter 1, the precise control of the PBGs width and wavelength positions can be achieved by thermal, electrical or mechanical approaches. Although these techniques are technologically well developed, there is an alternative approach to engineering the PBG. This approach requires the introduction of an additional component to the PhC, forming a multi-component PhC.

Multi-component PhCs have already been investigated in a number of recent papers, among which it is worthwhile to refer to the investigation of multi-component 1D PhC [1, 2]. The authors of paper [1] have theoretically analyzed the variations of the PBG's width and position with an increase of the number of components with various refractive indexes. However the same geometrical thickness was used for all the components in a multi-component structure despite the fact that it is well known that the thickness of each component significantly influences the optical properties of PhC. The authors of Ref. [2] have investigated theoretically and experimentally how the additional layer, introduced between $H$- and $L$-component, can
influence the reflectance spectrum position and leads to the narrowing of high-order PBG. As a result the analysis, performed in Refs. [1, 2], is related to specific structural types only and does not reflect the general behavior of multi-component PhCs.

In paper [3] more detailed investigations of 2D PhCs, containing intermediate layers on the surface of cylindrical pores, have been carried out. The authors have obtained the dependences of the PBG width and position from the additional interlayer thickness and its dielectric constant. They have considered a possibility to vary the lowest PBG position and width in 2D PhCs. It was shown that an interlayer with a thickness of only 1% of the lattice constant influences the band gap position quite significantly. In addition the insertion of the third component into the photonic structure decreases the PhC’s contrast and, consequently, the PBG width.

The authors of paper [4] succeeded in studying multi-component 3D PhC and have shown how to selectively manipulate with PBGs in multi-component PhC based on opal structure. For the description of optical characteristics with respect to the structural features more complicated model approaches, than that for 1D and 2D structures, were used. They have shown the possibility to control the stop-bands appearance, their width, and shift and ON/OFF switching by variation of additional layer’s thickness, permittivity and other factors in multi-component PhC.

In this Chapter, a three-component 1D PhC based on grooved Silicon was selected as the simplest example for calculations, as well as for demonstrating PBG modifications in both position and width, due to the introduction of an additional regular \( t \)-layer (Figure 3-1(d,e)). The optical properties of a three-component PhC structures have been analyzed using the GM approach and the TMM method. The introduction of a third component to a 1D PhC allows manipulation of the optical contrast to a high degree of precision by varying the thickness and refractive index of the additional layer. The approach can also be useful for finding the solution of the inverse problem, that is, for the interpretation of experimental reflection/transmission spectra for the photonic structures discussed here. Using the approach to decrease optical contrast in "Si-air" PhCs, omni-directional PBGs (ODBs) can be obtained. For some wavelengths, the limited number of PBGs vanish and are replaced by ultra-wide transmission bands (TBs) in the entire range of filling fraction. The fabrication of both band-pass and band-stop filters on a single PhC device enables optical manipulation at a variety of wavelengths. The suggested multi-component PhC model can be applied to
the design of any micro- and nano-structured semiconductor or dielectric materials for application across wide electromagnetic spectrum.

Figure 3-1: Schematic fragments of (a, b, c, e) two-component 1D PhC and (d) three-component 1D PhC with fixed value of lattice constant, a, and an additional t-layer. The thicknesses of H, L and t-layers are $d_H$, $d_L$, $dt$, accordingly.
3.2 Fabrication methods

The possible multi-component Si-based photonic crystal structures suitable for practical applications can be realized by, for example:

1. Fabrication of additional layers on the Si based structures using different deposition techniques
   or
2. Alteration of the existing layers formed on the Si side-walls, by either wet etching or reactive ion etching.

Several illustrative examples are discussed below.

**Example 1a.** Using a 1D PhC based on a "Si-air" structure, that is, grooved Si [5], and following the introduction of an additional SiO₂ layer, tuning of the PBG edge, either the main one or the high order PBGs [2], can be performed with a high degree of precision. This is because manipulation of the SiO₂ thickness for either 1D or 2D PhCs [3] can be performed very accurately by either thermal oxidation or by partial removal by wet etching using chemical reagents (Figure 3-2(a)).

In addition, SiO₂ is a solid material which is strongly attached to Si walls without an associated transition layer at the Si-SiO₂ interface. Lowering the optical contrast in a high contrast "Si-air" PhC enables the formation of a new PhC with a quasi-complete PBG. For this case, the sequence of layers can be \( n_{Si}/n_{SiO2}/n_{air} = 3.42/1.5/1 \).

**Example 1b.** Using a 1D PhC based on a multilayered "Si-SiO₂" structure, and introducing an additional layer of Si₃N₄, one can obtain a similar tuning of optical contrast, since in modern, thin-film technology, deposition of layers with tight thickness control ranging from nanometer (monolayer) to several micrometers and the optical characteristics required is possible to a high degree of precision. The sequence of layers in this case can be \( n_{Si}/n_{Si3N4}/n_{SiO2} = 3.42/2.2/1.5 \).

**Example 1c.** Using stain-etching for the fabrication of an additional porous layer on the Si side-walls, one can obtain a new photonic system with the desired optical properties and/or use the micro-porous layer as a matrix for sensing [6] (Figure 3-2(b)). Since the micro-porosity can be controlled, this ultimately can be used for tuning of the original 1D or 2D PhC. The sequence of layers in this case can be \( n_{Si}/n_{porSi}/n_{air} = 3.42/1.2-3/1 \).
Figure 3-2: Fabrication examples of the multi-component PhCs based on Si. Additional component obtained by a) thermal oxidation; b) stain etching; (c) infiltration with LC, and d) fabrication imperfection (here the corrugation of Si surface) as an additional t-layer.

**Example 1d.** Fabrication of an additional component in 1D and 2D PhCs, based on a “Si-LC” structure. In this case, the additional layer can be formed at certain orientations of nematic LC (e.g. commercially available LC E7 by Merck [7]) at the Si-LC interface [8], which is different from the orientation of the LC in the bulk. For example, at the interface, the orientation of the LC could be planar with an extraordinary refractive index $n_e=1.7$, while in the bulk, the LC could be in a homeotropic orientation with respect to the Si walls, which exhibits the ordinary refractive index $n_o=1.5$ (Figure 3-2(c)). For this case, the sequence of layers can be $n_S/n_e/n_o=3.42/1.7/1.5$.

**Example 2.** The additional $t$-layers can be formed by residual roughness with characteristic traces of the ribs left by the incompletely merged pores during electrochemical etching of Si [9] or the rough layer left after reactive ion etching. As the height of these residual ribs are comparable with the wavelength, they can be
Considered as anisotropic layers with the direction of the ribs along the etch depth. This rib system can be considered as an effective medium formed by a stack of parallel Si planes with air gaps between them with refractive indexes $n_{Si}$ and $n_{air}$ correspondingly (Figure 3-2(d)). The effective refractive indexes, $n_o$ and $n_e$, of the anisotropic layer can be described by formula for anisotropy of form [10]:

$$n_o^2 - n_e^2 = \frac{p(1-p)(n_{si}^2-n_{air}^2)^2}{(2-p)n_{air}^2+pn_{si}^2},$$

where $p$ is the rib system filling fraction. The values of $n_o$ vary from 2.8 to 3.0, while those of $n_e$ vary from 1.3 to 1.5 [11]. The following layer sequence can be considered in this case $n_{Si}/n_{rib}/n_{air}$ = 3.42/1.3-3/1.

3.3 Model of Multi-Component Photonic Crystal Structure

3.3.1 Modelling of the additional regular layers

A micro-structured Si structure with linear grooves [12] is considered here as a model for a basic 1D PhC structure, (see Figure 3-1(a, b)). The refractive index of Si for the high-refractive index, $H$, component in the mid-IR range is chosen as $n_{Si}=n_{hi}=3.42$. For the groove area, the refractive index of the low-refractive index, $L$, component, is considered to be $n_{air}=n_{li}=1$. In this case, the refractive index contrast is $n_{hi}/n_{li}=3.42/1$ and the structure can be considered a high-contrast PhC. As a result, only a small number of periods $N$ are needed to obtain a PBG with a reflectance of greater than 0.99. For comparison, the PhCs with other different contrasts, namely 3.42/1.5, 3.42/2.21, 2.21/1 and 1.5/1 are also considered here. We are looking for the common tendencies in PBGs caused by insertion of an additional regular $t$-layer with different refractive indexes, $n_t$, and thickness, $d_t$ (Figure 3-1(d)). During selection of $n_t$ values a particular attention is paid to two very common cases in practical applications i.e. when $n_t$ is varied between 3.42 and 1. In particular, in the case of $n_t=1.5$ we are dealing with an interlayer such as, for example, SiO$_2$ which can be deposited on Si walls with tunable thickness, while value $n_t=2.21$ we can use to take into account the roughness of Si walls (see Section 3.2).

In the latter case the optical characteristics of the roughness layer, $n_{rib}$, are equivalent to the effective homogeneous layer constructed from the combined parts of $n_{Si}$ and $n_{air}$. This assumption holds if the parameters of roughness (rout-mean-square height and autocorrelation length) are much smaller than the wavelength of the incident
light. The value of $n_r = 2.21$ for the porosity $p = 0.4$ [9] is taken as the average value of the refractive indexes of Si, $n_{Si}$ and air, $n_{air}$. The refractive index of the incoming and outgoing medium is $1$.

Calculation of the reflection spectra of 1D PhCs with $N$ periods and a filling fraction of Si, $f_{Si} = d_H/a$, where $a$ is the lattice constant, can be performed using the TMM [13]. An attractive feature of the method is the ease of introducing any number of additional layers at any point in the TMM's equation (see Chapter 2).

The Transfer Matrix $S_2$ used in calculations for a two-component 1D PhC structure, is given schematically by:

$$S_2 = ((I-M_H)(I-M_L))_N(I-M_H)$$  \hspace{1cm} (3.2)$$

for a three-component PhC matrix $S_3$, as shown in Figure 3-1(b), is:

$$S_3 = ((I-M_H)(I-M_L)(I-M_L))_N(I-M_H)(I-M_L),$$  \hspace{1cm} (3.3)$$

where $(I-M_H)$, $(I-M_L)$ and $(I-M_L)$ are the matrices of the $H$, $L$ and $t$-layers respectively.

### 3.3.2 Gap Map presentation

For each reflection spectrum calculated, the region of Normalized Frequency ($NF = a/\lambda$) where the reflection is greater than 0.99 was recorded on the plot. The PBG ranges obtained were then plotted, over a range of filling fractions, to give a plot known as a Gap Map (see Chapter 2 for more details). The result is displayed in Figure 3-3. For both GM and spectral calculations, the optical characteristics are presented in unitless dimensions of $NF$ and, therefore, can be applied to a wide range of structure sizes, including micro- and nano-structures.

The lattice constant, $a$, and the $t$-layer thickness, $d_t$, do not change, since $t$-layers with refractive index $n_t$ were introduced on both sides of the $H$-layer in the PhC structure, as shown in Figure 3-1(b). When generating $f_{Si}$, the value of $d_H$ for both the two-component and the three-component PhCs was kept the same. Thus, we can compare the two different PhC structures using the same $f_{Si}$ scale. As shown in Figure 3-1(c, e), $d_t$ decreases by $2 \cdot d_t$. When plotting the GM for this structure, not all filling fraction values $f_{Si}$ from 0.01 to 0.99 can be realized. The larger the value of $d_t$, the lower the maximum value of the filling fraction $f_{Si}$ that can be realized in the three-component PhC.
Figure 3-3: a) The lowest stop-band regions for GMs of three-component 1D PhCs, obtained from a two-component PhC with optical contrast 3.42/1 (curve 1) with an additional regular t-layer with various thicknesses $d_t$, shown, in units of $a$, by numbers beside the PBG areas. The value of $n_t=1.5$, number of periods $N=10$ and a normal incidence of light. For comparison, a two-component PhC with contrast 3.42/1.5, marked as 1.5, is also shown. The cutoff lines of the PBG regions correspond to $\max f_{\text{SI}}=0.74$ for $d_t=0.13a$, $\max f_{\text{SI}}=0.6$ for $d_t=0.2a$, $\max f_{\text{SI}}=0.46$ for $d_t=0.27a$, $\max f_{\text{SI}}=0.34$ for $d_t=0.33a$ and $\max f_{\text{SI}}=0.2$ for $d_t=0.4a$; b) Comparison of the lowest PBG areas for three-component and two-component PhCs with different optical contrasts (3.42/1, 3.42/1.1, 3.42/1.3 and 3.42/1.5), shown by numbers beside the curves.
In order to clarify this, consider an illustrative example with $a=3 \, \mu m$. This modifies the Si wall thickness $d_H = a f_{Si}$ from 0.03 to 2.97 $\mu m$. A $t$-layer thickness was taken, in this example, as $d_t = 0.4 \, \mu m$, corresponding to the parameter $d_t = 0.13a$. From Table 3-1, the GM for the three-component PhC can be calculated only up to the maximum value of the filling fraction, $max f_{Si}$, depending on $d_t$. In units of $a$, this covers the range from 0.03a to 0.47a.

**Table 3-1: The maximum value of the filling fraction, $max f_{Si}$, for various values of $t$-layer thicknesses, $d_t$, required for GM calculations of a three-component PhC with a lattice constant $a=3 \, \mu m$.**

<table>
<thead>
<tr>
<th>$d_t, \mu m$</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.6</th>
<th>0.8</th>
<th>1.0</th>
<th>1.2</th>
<th>1.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_t/a$</td>
<td>0.03</td>
<td>0.07</td>
<td>0.10</td>
<td>0.13</td>
<td>0.20</td>
<td>0.27</td>
<td>0.33</td>
<td>0.40</td>
<td>0.47</td>
</tr>
<tr>
<td>$max f_{Si}$</td>
<td>0.94</td>
<td>0.86</td>
<td>0.80</td>
<td>0.74</td>
<td>0.60</td>
<td>0.46</td>
<td>0.34</td>
<td>0.20</td>
<td>0.06</td>
</tr>
</tbody>
</table>

### 3.4 Engineering of the optical contrast

#### 3.4.1 Normal Incidence of Light

i) **Influence of $t$-layer thickness on Gap Map formation**

It is assumed that light is incident normal to the PhC structure and the angle $\theta = 0^\circ$ (Figure 3-1(a)). We select an $n_t$ value between 3.42 and 1, for example, $n_t = 1.5$. Note we are dealing with an interlayer such as SiO$_2$, which can be deposited on Si walls with tunable thickness.

Let us calculate the GM of the lowest PBG for the PhC ($N=10$) with $d_t=0.13a$ (Figure 3-3(a), curve 0.13a) and compare that with the GM for the original two-component PhC with $d_t=0$ (Figure 3-3(a), curve 1). As can be seen in Figure 3-3(a), $max f_{Si}$ restricts the formation of the PBG according to the data presented in Table 3-1. Hence, the GM was drawn for PBGs calculated over a range of filling fractions, $f_{Si}$, from 0 to 0.74. For other $d_t$ values, different GMs with corresponding cutoff lines at $max f_{Si}$, as shown in Figure 3-3(a), will be obtained. In Figure 3-3(a), the first PBG was considered for PhC structures with different $t$-layer thicknesses. A red shift of the PBG’s blue edge as $d_t$ increases is apparent from this figure. In the limiting case, as the $t$-layer thickness $d_t$ increases to the maximum value, the $L$ component tends to disappear.
and is totally replaced by the \( t \)-layer (Figure 3-2(e)). In this case, we obtain a two-component PhC again but with a different optical contrast of 3.42/1.5. Indeed, the cutoff line at \( f_S=0.74 \) intersects two SB areas for the first three-component PhC \( (d_t=0.13a) \) and for the second two-component PhC, but with a different contrast \( n=3.42/1.5 \). Similar trends are observed for other \( d_t \) values as shown more clearly in Figure 3-3(b) \( (d_t/a=0.33 \) and 0.4a).

**ii) Influence of \( t \)-layer refractive index on Gap Map formation**

Figure 3-3(b) enables the determination of the thickness of the additional layer with \( n_t=1.5 \) (at a value of \( f_S=0.2 \)) which forms a similar PBG to that in a two-component PhC with a specific value of \( n_L \). It can be seen that the PBG edges for \( n_L=1.1 \) and 1.3 for the two-component PhC intersect the PBG edges for the three-component PhC at \( f=0.2 \) with \( d_t=0.13a \) and 0.27a. As a result, we observe an impact on the PBG areas of the three-component PhC, demonstrating the possibility of manipulating the optical contrast by changing the thickness of the additional regular layer in the PhC structure. In other words, the \( d_t \) value provides an equivalent value of \( n_t^{equ} \) for a two-component PhC with the same \( n_H \) value. However, in our case, the range of possible \( f_S \) values for PhC fabrication decreases significantly. This in turn leads to a reduction of the regions of PBGs on the GM. For example at \( d_t=0.33a \), the values of \( f_S \) range from 0 to only 0.34 (Figure 3-3(a)). It is worth mentioning that the remaining portion of the PBG's on the GM is still comparable to that for the original two-component PhC and, indeed, they remain the widest PBGs inside this range of \( f_S \).

In order to prove the equivalency concept demonstrated in Figure 3-3(b), the three-component “Si-SiO\(_2\)-air” PhC structure was fabricated using optical lithography and Deep Reactive Ion etching of (100)Si (see Chapter 2 for details) followed by thermal oxidation at 1000°C in order to grow a smooth oxide layer of thickness \( d_{Si}=580 \text{nm} \) on top of Si side walls. The reflection spectrum of the obtained structure was measured in mid-infrared range from 2000 to 7000 cm\(^{-1}\) using FTS 6000 FTIR spectrometer in conjunction with a UMA IR microscope. Note, the reduction of the maximum \( R \) intensity as well as a smoothing of the “IT”-shape of PBGs in the experimental spectra (Figure 3-4) is due to the “shading” effect from the substrate of the structure and cone-like shape of the light beam (see Section 2.4). The simulations of the obtained experimental spectrum have demonstrated that the positions and width of the PBGs of the fabricated three-component structures are the same as for the same
structure without the third component but instead infiltrated with some unknown filler with refractive index \( n_i = 1.185 \) (Figure 3-4). Obviously, manipulation of the PBG parameters by changing the thickness of the additional layer is the preferred route. Apart from the thickness, one can also vary the \( n_i \) value of the additional layer and, by doing so, obtain the dependence of \( n_L^{eq} = f(n_i) \). An example of this for values of \( n_i = 2.2 \) and 3 is shown in Figure 3-5, along with results obtained earlier for \( n_i = 1.5 \). As can be seen from this figure, for the parameters of \( n_i \) selected, the range of \( n_L^{eq} \) can be varied from 1.1 to 2.2.

![Figure 3-4: Equivalency of the experimental PBGs of three-component PhCs with \( N=4, a=4\mu m \) and \( f_{Si}=0.157 \) with additional layer thicknesses of the \( SiO_2, d_{SiO_2}=580nm \) and simulated PBGs of the same PhC without \( SiO_2 \) component, but infiltrated with some unknown filler with refractive index \( n_L=1.185 \).](image)

The examples illustrate the influence of \( n_i \) and \( d_i \) on PBG formation, since both of these parameters can be altered technologically. For example, the refractive index of the additional layer can be changed keeping the thickness constant, or the additional layer with a constant value of \( n_i \) can be fabricated with different thicknesses using various deposition techniques from the gas or liquid phase, or by thermal oxidation. We conclude that using a multi-component PhC is a viable alternative technique for the
alteration of the optical contrast of PhCs and, therefore, for tuning the position and width of PBGs in the reflection/transmission spectra of these structures.

Let us analyse what happens to PBGs of high order following the introduction of an additional layer using the GM of PBGs in the range of $NF = 0-2.5$. As can be seen from Figure 3-6, the introduction of the $t$-layer with different $d_t = 0.13a$ and $n_t = 1.5$ results in:

- a decrease in the area of every PBG region,
- a red shift of the PBG regions with respect to the original two-component PhC.

![Figure 3-5: The dependence of $n_{eq}$ (which is equivalent value for a two-component PhC) versus $d_t/a$ for three-component PhC with a $t$-layer of thickness, $d_t$, and refractive index, $n_t$, (the numbers beside the lines) and $f_{si} = 0.2$.](image)

A decrease of the PBG width with an increase in the $t$-layer thickness can also be seen in Figure 3-3(a) for the lowest PBG in more detail. Similar behavior was observed earlier in the GM of PBGs in a two-component PhC as $n_t$ increased [12, 14]. Thus, the introduction of the $t$-layer has a similar effect to the substitution of $n_t$, i.e. it serves to decrease the optical contrast or, in accordance with Ref. [3], to decrease the effective dielectric constant. As can be seen from Figure 3-6, the size of the high-order SBs regions for three-component PhCs differs from that in ordinary PhCs. In the range of $NF$ values from 1 to 1.5, a suppression of high order PBGs takes place. The
suppression of stop-bands and their replacement with transparent regions was investigated earlier for multi-layer films in Refs. [15-17]. A similar narrowing effect was also observed in our case for the high-order PBG realized for Si-based PhC, as shown in Figure 3-6. One possible explanation of this effect is that the third component is acting as an antireflection coating, suppressing the high order PBGs. This interesting effect will be a subject for investigation in the next Section 3.5.

Figure 3-6: Influence of the t-layer \((d_t/a=0.13a)\) on the shift and decrease of PBG regions of high order in the region \(NF=0\)-2.5.

Furthermore, we have developed a series of maps with the lowest PBGs for the consequent two-component PhC by changing the optical contrast of the original two-component PhC from 3.42/1 to 3.42/1.5 and letting \(n_t=2.2\) (see Figure 3-7(a)). As shown earlier, we obtain tuning of the optical contrast by introduction of the additional \(t\)-layer. Using a smaller value of \(n_t=1.7\), we have obtained a much smaller shift of the blue edge of the PBG as seen in Figure 3-7(b). In summary, we demonstrate, once again, the possibility of tuning the optical contrast of a three-component PhC by varying either the thickness or the refractive index of the \(t\)-layer.
Figure 3-7: (a) Gap maps of a two-component 1D PhC with contrast $n=3.42/1.5$ (curve 1.5) with added $t$-layers of different thicknesses $d_t$, shown beside the curves in units of $a$, and with refractive index $n_t=2.2$. The GM with contrast $n=3.42/2.2$, the SB region marked as 2.2, is also presented for comparison. (b) Gap maps of a two-component 1D PhC with contrast $n=3.42/1.5$ (curve 1.5) with added $t$-layers of different thicknesses with a refractive index $n_t=1.7$. The GM with contrast $n=3.42/1.7$, marked as 1.7, is presented for comparison. The calculation is performed at a normal incidence of light with the number of periods $N=10$. The cutoff lines are the same as in Figure 3-3. Note that only the lowest stop-band areas are shown for simplicity.
It is worth noting that the additional layer, with a definite optical thickness, \( n_t d_t \), introduces a contribution to the overall interference of the reflected wave, but it does not have a damaging effect on the \( R \) value in the PBGs. As can be seen from Figure 3-3 and Figure 3-7, the reflection coefficient is still equal to 0.99, since this value is still the criterion for PBG formation. However, this is a rough estimate. We will consider further how under these conditions the quality of the reflection bands is changed within the PBGs, because different perturbation factors often result in a decrease in the absolute value of the reflection coefficient in the PBG to \( R=0.9 \) or even less. In addition, changing the shape of the PBG can increase the noise level and other types of band degradation can also occur. Typically, these effects are better seen in transmission mode of the lowest PBG. The spectrum for a contrast of 3.42/1 and a filling fraction of \( f_S=0.23 \), corresponding to the quarter wavelength thickness of the layers, is shown in Figure 3-8 with the smallest transmission value of \( T=10^{-11} \). The introduction of a \( t \)-layer

![Figure 3-8: Transmission spectra shown for the lowest SB areas for a two-component PhC with an optical contrast of 3.42/1 (curve 1) and 3.42/1.5 (curve 1.5) and for three-component PhCs with an additional \( t \)-layer of \( n_t=1.5 \) and thicknesses of \( d_t=0.13a \) and \( 0.27a \). Calculations were performed at a normal incidence of light with \( f_S=0.23 \) and \( N=10 \).](image-url)

with \( d_t=0.13a \) increases \( T \) to \( 10^{-10} \), while this increases to \( T=10^{-7} \) at a lower PhC optical contrast of 3.42/1.5. Therefore, the introduction of the \( t \)-layer affects the properties of 54
the lowest PBG, not as a degradation factor, but as a characteristic tendency to decrease the optical contrast of the PhC.

3.4.2 Oblique incidence of light: Omni-directional properties

It is known [18] that the omni-directional band in the gap map is determined by the overlapping regions of the stop-bands obtained for different angles of incidence and various polarizations of light. Using the TMM, reflection spectra can be obtained for different deviation angles, $\theta$, of the wave-vector from the normal (see Figure 3-1(a)), over a range of $\theta$ from $0^\circ$ to $90^\circ$ for TM- and TE-polarizations, where TM and TE are the Transverse Magnetic and Transverse Electric polarizations, respectively.

![Figure 3-9](image)

**Figure 3-9:** Gap maps, demonstrating the formation of an ODB region (the striped area), as a common area formed by the overlapping of PBG regions at different angles of incidence. Angles of incidence are indicated by the number beside the curves. The contrast was 3.42/1 and the additional layer had $n_f=1.5$ and a) $d_i=0.2a$, b) $d_i=0.27a$, c) $d_i=0.33a$ and d) $d_i=0.4a$. ODB regions for a two-component PhC with contrast of 3.42/1.5 (grey region) and for three-component PhC (striped region) are shown for comparison in (d).
The width of the PBGs for TE-polarization increases with an increase in $\theta$, while for TM-polarization it decreases. As a rule, it is necessary first to be sure that the PBGs for TM-polarization have a common area for different $\theta$ and then to identify this area as the ODB. Let us perform the GM calculation for an optical contrast of 3.42/1 and number of periods $N=10$. The ODB region does not form for this optical contrast [19]. The additional introduced layer is of thickness $d=0.2a$ and refractive index $n=1.5$ with angle of incidence change from $\theta = 0^\circ$ to a maximum value of $85^\circ$ with a step size of $5^\circ$. Figure 3-9(a) shows that the photonic band gaps obtained for TM-polarization overlap at different angles $\theta$. Note that, for clarity, only a few angles viz. $\theta = 0^\circ, 70^\circ, 75^\circ, 85^\circ$ are shown on Figure 3-9(a). They form a common ODB area, shown by the striped area.

![Figure 3-10: The width of ODBs versus filling fraction (calculation from Figure 3-9).](image)

This region is formed in the three-component PhC under consideration over a range of filling fractions, $f_{Si}$, from 0.25 to 0.6, causing the position of the ODB region to vary from 0.22 to 0.39 in units of $NF$. Note that the cutoff line of the PBG is located at higher values of $f_{Si}$ than are necessary for formation of the ODB (see Figure 3-9(a)), therefore the parameter $max f_{Si}=0.6$ does not limit the $f_{Si}$ values for a PhC with an ODB. Figure 3-10 demonstrates the dependence of the ODB width ($\Delta NF_{ODB}$) on $f_{Si}$ from which the region of formation of the ODB can be deduced for $f_{Si}$ values from 0.22 to 0.6.
with a maximum $\Delta N_{F_{\text{ODDB}}}=0.024$ at $f_{\text{SI}}=0.31$. As pointed out in Ref. [20], this value does not correspond to $\lambda/4$ layers, corresponding to $f_{\text{SI}} = 0.23$ for the PhC with contrast $3.42/1$, and shifts to higher values of $f_{\text{SI}}$ due to the necessity of taking into account overlapping of the PBG at different angles of incidence and different light polarizations.

**Figure 3-11:** Transmission spectra $T$ and ODB width (filled rectangles) shown for the first PBG at incident angles of $0^\circ$ and $85^\circ$ for: a) three-component PhC (denoted as 3comp) with an additional layer $n_r=1.5$ and $d_r=0.2a$ and two-component PhC (denoted as 2comp) with optical contrast $3.42/1$ without ODB region (filling fraction $f_{\text{SI}}=0.3$); b) three-component PhC with an additional layer $n_r=1.5$ and $d_r=0.27a$ and two-component PhC with contrast $3.42/1.2$ ($f_{\text{SI}}=0.3$); c) three-component PhC with $n_r=1.5$ and $d_r=0.33a$, $f_{\text{SI}}=0.3$ and two-component PhC with contrast $3.42/1.4$ ($f_{\text{SI}}=0.3$); d) three-component PhC with additional layer $n_r=1.5$ and $d_r=0.4a$ and two-component PhC with contrast $3.42/1.5$ ($f_{\text{SI}}=0.2$). The dashed line corresponds to the level of $T_{\text{PBG}}=0.001$ (or $R_{\text{PBG}}=0.999$).
As mentioned above, introduction of the \( t \)-layer with \( d_t = 0.2a \) is in fact equivalent to an increase of the \( n_\ell \) value to \( \approx 1.2 \). This is higher than the minimum value of \( n_\ell = 1.1 \), which allows the appearance of ODBs in high optical contrast PhCs [18]. However, in practice it is problematic to find a suitable filler with a refractive index \( n_i = 1.1-1.2 \) for impregnation into a PhC. Therefore, introduction of a \( t \)-layer is the preferred approach in this case.

Let us now use another value of \( d_t = 0.27a \) for calculating the GM (see Figure 3-9(b)) and plot two stop-bands only, which determine the ODB areas for TM-polarization and incident angles in the range 0° to 85°. As shown in Figure 3-9(b), and in accordance with Table 3-1, the cutoff line is drawn at a value of \( f_{St} = 0.46 \) and actually truncates the ODB. At the same time, the maximum \( \Delta N F_{ODB} \) increases to 0.043. The increase of \( d_t \) to a value of 0.33a leads to a lowering of the cutoff line (see Figure 3-9(c)), as expected, and to a simultaneous increase in \( \Delta N F_{ODB} \) (Figure 3-10, line 0.33a). A further increase of \( d_t \) to 0.4a significantly decreases \( \Delta N F_{ODB} \) (Figure 3-10, line 0.4a). Since the introduction of layer \( d_t \) is equivalent to a reduction in the optical contrast of the PhC, at the limit of this case we should obtain a PhC with contrast 3.42/1.5. Indeed, as can be seen in Figure 3-9(d), the ODB area for the three-component PhC, shown by the striped area, practically overlaps the ODB area for the two-component PhC, the grey area, within the limit of the permitted range of \( f_{St} \).

In order to demonstrate the qualities of PBGs in transmission \( T \)-spectra, \( T \)-spectra were calculated using a filling fraction \( f_{St} = 0.3 \) from Figure 3-10, for which maximum ODB width can be achieved. Calculated transmission spectra are presented in Figure 3-11. For a sample with \( d_t = 0.4a \), we can select a value of \( f_{St} = 0.19 \) due to the cutoff line. The spectra obtained demonstrate overlapped regions of stop-bands for TM-polarization and two incident angles of 0° and 85°. In producing this plot, transmission spectra were calculated over the total range of possible angles of incidence with a step size of 5°, but these were omitted from the plot for clarity.

Figure 3-11(a) shows spectra for comparison from a two-component PhC with a contrast of 3.42/1. The structure does not form an ODB, since there is no overlapping of the PBGs for angles of incidence of 0 and 85°, see the curves corresponding to 0° and 85° for the two-component case on the plot. At the same time, introduction of a \( t \)-layer with \( d_t = 0.2a \) results in overlapping of the PBGs and leads to the formation of an ODB area. A similar effect is observed for other ODB areas with different \( t \)-layers (see Figure 58).
As can be seen from all the plots presented in Figure 3-11, the introduction of the \( t \)-layer into ordinary two-component PhC does not decrease the width of the ODB area.

### 3.5 Formation of Infrared Regions of Transparency

An analysis of the GMs of the PBGs for the three-component PhC revealed a red shift, as well as a decrease of the PBG area, with respect to the original ordinary two-component PhC, with an increase of the \( t \)-layer thickness, \( d_t \) (see Figure 3-6). Further investigation has revealed that for the small number of period \( N<10 \) the high order PBGs are not only suppressed but can be vanished in a wide frequency and entire filling fraction range.

#### 3.5.1 Suppression of Photonic Band Gaps

In Figure 3-12 we compare the GMs over a wide range of \( NF \) for an ordinary two-component “Si-air” PhC (grooved Si) with the number of periods \( N=5 \) and for multi-component PhC based on the same “Si-air” structure after introduction of the regular \( t \)-layer with thickness of \( d_t = 0.10a \). It is apparent that the lower PBGs are least affected by the addition of the \( t \)-layer, retaining a similar area and experiencing a negligible red shift in frequency. At the same time, inspection of the high-order PBGs over the entire range of \( NF \), reveals regions of frequency, or equivalently wavelength, for which PBGs are suppressed, with \( R<0.99 \). Note that the SBs determined for the original “Si-air” PhC structure are not suppressed over the entire \( NF \) range (Figure 3-12). A detailed examination of the suppressed high-order PBGs in these frequency regions reveals that PBGs are not only significantly suppressed, but can actually disappear, with \( R=0 \). It is obvious that the regions of transmission could appear in these regions of frequency instead. Let us calculate a set of transmission spectra for a multi-component 1D PhC with a \( t \)-layer thickness of \( d_t =0.1a \) over a range of \( f_{St} \) values from 0.08 to 0.1 with a step size of \( \delta f_{St}=0.001 \) (Figure 3-13(a)). Indeed, the transmission bands are formed between the suppressed PBGs, with \( R \) less than 0.99. It is clear from Figure 3-13(a) that the TB’s range is constant for filling factors, \( f_{St} \), in the range 0.083 to 0.093, that is, with a change in the filling factor of \( \Delta f =0.093-0.083=0.01 \). Additional detail can be seen in Figure 3-13(b), where the transmission range is expanded across the range of transmissions from 0.97 to 1 in order to increase the clarity of the diagram. As shown in Figure 3-13(b), the width of the TBs is also dependent on the selection of
the cutoff transmission value. For example, if a cutoff transmission was chosen as 0.995, then the TBs within a narrow range of $NF$ will appear narrower and less uniform than those for a cutoff level of 0.99. The choice of an appropriate cutoff level is an important design criterion when engineering practical device structures. Let us consider an example of the design of a real band-pass filter based on the three-component PhC model from Figure 3-13. Suppose the lattice period, $a$, is 3000 nm and the Si-wall thickness, $d_{W}=f_{Si}a$, is 260 nm, corresponding to a filling factor $f_{Si}=0.087$. According to Figure 3-13(b), such an optical filter has a wide pass-band with bandwidth of 0.36 $NF$ (350 nm) centered at $NF=1.7$ or a wavelength $\lambda=a/NF=1760$ nm for a cutoff level $T=0.99$. From Figure 3-13(a) the filling factor deviation $\Delta f_{Si}$ is up to 0.03, which corresponds to the possible Si wall thickness deviation $\Delta d_{W}=30$ nm for this particular example filter.

**Figure 3-12:** GMs for a two-component "Si-air" PhC (light regions) and for a multi-component PhC with $n_{r}=1.5$ and $d_{r}=0.10a$ (dark regions) over a wide range of $NF$; $\max f_{Si}=0.80$. The calculations are performed at normal incidence of light with number of periods $N=5$. 60
Figure 3-13: The transmission spectra $T$ for multi-component PhC with $t$-layer refractive index $n_t=1.5$ and thickness $d_t=0.10a$ for (a) $f_n=0.08...0.1$. (b) The same as in figure (a) shown for clarity in expanded transmission scale for $f_n=0.087$. The calculations are performed at normal incidence of light with number of periods $N=5$.

3.5.2 Influence of the additional component thickness

Now that we have established the general criteria for TB formation, we can plot a map of the regions of transparency (RTs) for the multi-component PhC by analogy with the GM for PBGs [14, 19]. In order to avoid plotting very narrow peaks with high transmission, $T>0.99$, from the spectrum in Figure 3-13(b) (see, for example, peaks at $NF=1, 2.2, 2.4$) we need to define a minimum range of $\Delta NF>0.01$, which provides transmission values $T>0.99$. Removal of the narrow regions, by defining $\Delta NF<0.01$ greatly improves the clarity of the TBs. In Figure 3-14(a) the map of TBs is demonstrated with the GM, simulated for the “Si-air” PhC structure with additional component with refractive index $n_t=1.5$ and thickness $d_t=0.13a$. It is apparent, that the TB regions are located between the SBs areas of the corresponding PhC structure. Note the total suppression of high order SBs over a range of $NF$ from ~1.1 to ~1.5. This $NF$ range also contains the widest TBs. This is also confirmed by the transmission
spectrum, shown below in Figure 3-14(b). Therefore, we conclude that the third layer in 1D PhC structure can be treated as an antireflection layer by analogy with multilayer dielectric coatings.

![Image](image_url)

**Figure 3-14:** a) The GM of stop-bands \((R>0.99)\), denoted as SBs, and map of transmission bands \((T>0.99)\), denoted as TBs, for the multi-component PhC with \(n_t=1.5\) and \(d_f=0.13a\). b) The transmission spectrum \(T\) for the same multi-component PhC for \(f_{si}=0.117\). The calculation is performed at normal incidence of light with number of periods \(N=5\).

It should be noted that the PBGs, also referred here as SBs, determined for the ordinary PhC structure, shown in Figure 3-12, are not suppressed over the whole \(NF\) range and, therefore, originally have no wide TBs in this range.
Let us now analyze the changes that occur in these wide TBs, when the thickness of the additional t-layer is varied, using maps of the transparency regions. For this purpose, maps of TBs for the three-component PhC with t-layer thicknesses $d_t = 0.20a$ and $d_t = 0.33a$ were calculated (Figure 3-15). The calculation procedure, used to
determine the TBs and the form of their graphical representation are the same as that described earlier.

It is worth noting that, for the PhC with $d_l=0.20a$, the TBs exhibit a different behaviour than for the case of $d_l=0.13a$. The widest TBs disappear between 1.1 and 1.4, reappearing again in two NF regions, viz. from 0.5 to 1.1 and from 2.3 to 2.6. As shown before, these features were not observed for the ordinary two-component PhC with optical contrast $3.42/1$ (see Figure 3-12(a), light grey curves). Moreover, as expected, for an additional layer thickness of $d_l=0.33a$, we can already see the formation of three regions with wide TBs over the same NF range. Thus, an increase in the $t$-layer thickness results in an increase in the number of TBs. Therefore, by changing the thickness values of $t$-layer we can manipulate with width and number of TBs in Si PhC device.

3.5.3 Influence of the oblique incidence of light

Based on the preliminary calculations performed in Section 3.5.2, we have successfully demonstrated how the thickness of the $t$-layer is affecting the formation of the regions of transparency in multi-component Si photonic crystal. The next important issue, which needs further investigation, is the impact of oblique incidence of light on TBs. As it was demonstrated earlier, the PBGs cannot be obtained at certain angles of incidence of light for 1D "Si-air" PhC structures, regardless of the filling factor $f_S$. In Section 3.4 we have shown, that by lowering the effective optical contrast (e.g. from high to medium) due to introduction of the additional components, one can obtain the omni-directional PBGs in initially high-contrast structures. The calculated omni-directional PBGs for multi-component PhC structure have even larger width, than those for the equivalent two-component structures with medium optical contrasts, for both TM- and TE-polarizations of light.

Let us consider now the multi-component "Si-air" PhC system with the additional $t$-layer of the thickness $d_l=0.2a$. A detailed analysis have shown that an increase of the angle of incidence of light, $\theta$, does not affect significantly the formation of TBs, which are experiencing only a blue shift in an entire range of $f_S$. At the same time, a large increase of the angle of incidence ($\theta>50^\circ$) leads to the widening of TBs for TM-polarization and their narrowing for TE-polarization. On the contrary, as was demonstrated in the past, the width of the SBs for TE-polarization increases with an
increase in $\theta$, while for TM-polarization it decreases [19]. Therefore, we can expect that at certain conditions the wide SBs for TE-polarization may overlap with the wide TBs for TM-polarization. The overlapping regions determine the regions of frequency for

Figure 3-16: The GM of SBs ($R>0.99$) for TE-polarization (light regions) and map of TBs ($T>0.99$) for TM-polarization (dark regions) for the multi-component PhC with $d_i =0.2a$ in a wide $f_{Si}$ range (a) and in limited $f_{Si}$ range (b). The calculation is performed at angle of incidence $\theta = 60^\circ$. 
which a multi-component PhC structure is totally transmitting the TM-polarized light and totally reflecting the TE-polarized light, and, therefore, this structure is acting as a highly efficient polarizer. In Figure 3-16(a), we demonstrate the GM, calculated for $\theta=60^\circ$ for TE-polarization, which is compared to the map of TBs, calculated for the same angle $\theta$ but for TM-polarization of the incident light. It is apparent from Figure 3-16(a) that the TBs have partially overlapped with SBs in a whole range of $f_{Si}$. For clarity, the same maps are demonstrated in the limiting range of $f_{Si}$ and $NF$ in Figure 3-16(b). It is clearly seen, that the overlapped regions can reach the width up to 0.05 $NF$ for certain values of $f_{Si}$. For the example considered here, $a=3$ $\mu$m, this width value is equivalent to approximately 60 nm. In order to demonstrate the overlapped regions in details, as well as to show the qualities of the obtained TBs in transmission spectra, the $T$-spectra for both polarizations were calculated using a filling factor $f_{Si}=0.18$ (Figure 3-17). The overlapped regions for both polarizations correspond to the maximum value of $T$ for TM-polarization and the minimum value of $T$ for TE-polarization. It is also apparent, that the overlapped regions (with $T>99\%$) demonstrate a negligible number of ripples on the top.

![Figure 3-17: The T spectra for $f_{Si}=0.18$ calculated for the multi-component PhC with $d_i=0.2a$ at angle of incidence $\theta=60^\circ$. The formation of TB for TM-polarization and SB for TE-polarization at $NF=1.62$ demonstrates the transformation of the PhC into TM-polarizer in transmission mode and TE-polarizer in reflection mode.](image)

We conclude that the introduction of the additional, regular layer into a high optical contrast 1D PhC, like for example grooved Si, results in the appearance of wide
regions of transparency for TM-polarization for an oblique incidence of light. Using an appropriate design a photonic crystal polarizer, based on grooved Si, can be fabricated for efficient operation with $T > 99\%$ for TM-polarization and $R > 99\%$ for TE-polarization in a specific wavelength regions.

The proposed model of in-plane Si-based multi-component PhC allows realization of the highly compact integratable broadband polarizer on Si chip. Comparing to the other typical commercial non-integratable polarizer solutions the multi-component PhC polarizer demonstrate an outstanding wide angular field of $30^\circ$ and high extinction ratio of about $30\text{dB}$. However, further theoretical and experimental investigation required in order to understand how the dispersion of Si and insertion losses may influence the polarizing characteristics.

3.6 Photonic Crystal ultra-wide pass-band filter

Let us use the suggested in the previous Section GMs of TBs for the fabrication of the real band-pass optical filter with wide bandwidth operating in a mid-infrared (MIR) wavelength range. In order to introduce the third component into original two-component structure, we exploited thermal oxidation of the grooved Si structures. While other complex and more expensive deposition techniques, such as chemical vapour deposition or sputtering, can be used to deposit dielectric layers, thermal oxidation of Si has the advantage of having a better growth isotropy, especially for narrow, deep trenches and precise control of the grown thickness. Also the fundamental limitations of fabricated Si based devices, such as high roughness and corrugation of the etched Si surfaces, can be overcome by oxidation smoothing (see Section 3.2). In the course of the model calculations we have to pay attention to the following important issues. Firstly, owing to the strong absorption band of $\text{SiO}_2$ around $9 \mu\text{m}$ in MIR range of spectra, the imaginary part of $\text{SiO}_2$ refractive index, $n_{\text{SiO}_2}$, has been taken into account [21]. It was found that this absorption band does not coincide with total transmission regions in multi-component PhC with lattice constant, $a$, less than $5 \mu\text{m}$. Secondly, during thermal oxidation the 44% of oxide thickness is formed at the expense of Si wall while the remaining 56% of the oxide grows outside in the air [2]. Therefore, the maximum $f_{\text{Si}}$ of resulting three-component device will be reduced by the value $\Delta f_{\text{Si}} = (2\cdot0.44\cdot d_{\text{SiO}_2})/a$. For fabrication convenience let us use the original grooved Si structure with a lattice period $a = 4 \mu\text{m}$ and the thickness of the additional component.
Only three “Si-air” paired layers with $N=3$ are needed in order to demonstrate the SBs formation and their further replacement with TBs, making the device extremely compact and potentially low loss. An in-plane design, in which the SBs structure is etched into the Si substrate, allowing the incorporation of optical fibre in-plane, eases the integration process and facilitates the construction of a high-quality filter. The reflection, $R$, spectra for the original (two-component) structure in the range of filling fractions from 0.25 to 0.33 are demonstrated in Figure 3-18(a). The device calculated can operate as a reflecting filter, with a wide SB centred at $\lambda_c=0.85\ NF$.

![Figure 3-18](image)

**Figure 3-18:** 3D representation of (a) flat-top SB centred at 0.8NF in the range of filling fractions $f_{Si}=0.25-0.33$ before oxidation and (b) flat-top pass-band centred at the same frequency calculated for the same device after oxidation in the range $f_{Si}=0.10-0.17$. The thickness of SiO$_2$ is $d_{SiO2}=0.18a$.

In Figure 3-18(b), the transmission spectra, $T$, are demonstrated for the structure after thermal oxidation over the new range of filling fractions $f^*_{Si}=f_{Si}-\Delta f_{Si}$, varying from 0.10 to 0.17. It is apparent from the $T$ spectra that the regions of high transmission
(T>99%) have widened and totally replaced the SB. The obtained structure can now operate as a band-pass filter centred on the wavelength, $\lambda_c$.

Figure 3-19(a) shows the maps for the discussed structure calculated in a wide range of $f^*_S\Delta f^*_S$ from near-infrared to mid-IR spectral ranges. As can be seen for this figure, the introduction of the regular SiO$_2$ layers in the device has affected the formation of SBs significantly. The limited number of high-order SBs have vanished in a full range of $f^*_S$ over two wavelength regions (around 4 μm and 1.5 μm). At the same time the regions of high transparency with $T>99\%$ (black regions) have become significantly wider in the same wavelength regions. It is also clear that the widest TBs are observed for the filling factor values less than 0.5, which actually corresponds to more realistic structures. According to TB’s map the final device should have a filling factor $f^*_S=0.145$ and, therefore, the final Si-wall thickness, $d^*_f=f^*_S\Delta f^*_S=0.58$ μm. In the Figure 3-19(b) the same map is presented in the limited range of $f^*_S$ from 0.075 to 0.2 in order to study the TBs and SBs for the proposed structure in details. It is obvious that the filling factor deviation, which corresponds to the pass-bands of the same bandwidth and centered at the same wavelength $\lambda_c$, is up to 0.03. Thus, the fabrication tolerance (photolithography error) can be easily estimated from the proposed TB’s map, which constitutes 120 nm for the particular demonstrated example filter.

For the fabrication of the original grooved structure we used a fabrication process that was described in details in Chapter 2. The anisotropic chemical etching of (110)Si by KOH was used for the initial step. The depth of etching was 15 μm. Following this, grooved structure was thermally oxidized at the temperature $T=900$ °C for 120 min in order to grow an oxide layer of the thickness $d_{SiO_2}=0.18\alpha=720$ nm on the top of Si side-walls (Figure 3-20). The spectroscopic ellipsometer Ellipse 1891 developed in the Institute of Semiconductor Physics of the Siberian branch of the Russian Academy of Sciences was used for thickness control of the SiO$_2$ layers on witness samples. Measurements were performed at an angle of light incidence $\phi_0=70^\circ$ over the photon energy range 1.5-5.0 eV. The thickness of thermally grown oxide layer and information about the refractive index were obtained by fitting the measured data to multi-layer model calculations. The $R$ and $T$ spectra measurements have been performed using an FTS 6000 FTIR spectrometer in conjunction with a UMA IR microscope (see Chapter 2 for details). The aperture of the focused IR beam was 15×15 μm$^2$ and the spectral resolution was 8 cm$^{-1}$. A golden mirror was used as a 100% reference for
measurements of reflection spectra. All measurements have been performed for normal incidence of light.

Figure 3-19: (a) The GM of SBs with R>0.99 (light regions) and map of TBs with T>0.99 (dark regions) calculated for fabricated filter based on PhC structure (air-$\text{SiO}_2$-$\text{Si}$-$\text{SiO}_2$-air)$^N$ with $N=3$ for mid-IR. (b) The same maps, demonstrated in the limited range of $\lambda$ and $f_\text{Si}$ for clarity. The dispersion of $\text{SiO}_2$ in MIR range and normal incidence of light $\theta=0^\circ$ are taken into account during calculations.
Figure 3-20: SEM image of photonic crystal filter based on grooved Si with thermally grown SiO$_2$ of thickness $d_{SiO_2}=0.72\, \mu m$. The lattice period $a=4\, \mu m$.

Figure 3-21: Experimental (dashed line) and calculated (solid line) (a) $R$ and (b) $T$ spectra of the band-pass filter based on PhC structure (air-SiO$_2$-Si-SiO$_2$-air)$^N$ with $N=3$ demonstrate the transformation of the SBs at 3.5 $\mu m$ and at 4.8$\mu m$ into the TB at the wavelength $\lambda_c=4.2\, \mu m$.  

71
Figure 3-21 shows the experimental $R$ and $T$ spectra in comparison with the simulated ones. Apart from some excess losses, which may be due to optical scattering, there is good agreement between experiment and calculation. We note that the original grooved Si structure has the SBs centred at 3.5 μm and 4.8 μm. Thus, the original device is acting as a stop-band filter (Figure 3-21(a)), while after thermal oxidation these SBs have been replaced with ultra-wide TB with bandwidth of 1400 nm in the range of wavelength from 3.4 μm to 4.8 μm. The obtained device can now operate as band-pass filter (Figure 3-21(b)). To our knowledge this is the first report of the broadband band-pass filter with flat-top characteristics which can be integrated on Si chip. The utilization of the thermally grown SiO$_2$ for the fabrication of the multi-component PhC device has resulted in the appearance of the negligible number of ripples (with depth up to 4-5%) on the otherwise flat-top transmission. Therefore, the fabricated band-pass filter can provide an ultra-wide transmission of 95-96% centred at 4.2 μm.

3.7 Summary

Utilisation of a three-component photonic crystal by the introduction of an additional layer to a two component structure, while leaving the lattice constant unchanged, provides a suitable model for designing a new type of photonic crystal. Use of a GM allows visualization of the transformation of the PBG areas caused by converting a two-component PhC to a three-component PhC by the addition of the new layer. The introduction of the third component to the 1D PhC allows variation of the PBGs areas of the three-component PhC and, therefore, engineering of the optical contrast of the original two-component PhC. This is achieved, not by filling its air channels, but by selecting either the thickness or refractive index of the third layer. However, in this case, we sacrifice the range of possible $f_{Si}$ values for the formation of stop-bands and SB’s area. The widest SBs are observed for this restricted range of possible $f_{Si}$ values. Using the approach suggested for decreasing the optical contrast in photonic crystals, omni-directional bands can be obtained in a high-contrast Si-air periodic structure. A number of simulated models of three-component 1D photonic crystals are described, some of which may have practical applications.
The principle of suppression of the PBGs and replacing them with TBs is demonstrated for a high contrast 1D PhC with the introduction of an additional \( t \)-layer. By varying the thickness of the \( t \)-layer, the width and the number of the TBs can be altered. The TBs obtained numerically show a high transmission value (>99%) and a substantial band width in the infrared spectral range. The GM approach was used to generate the map of transmission bands in order to observe the effect in the entire range of Si filling factor and in a wide wavelength range. The generated maps of TBs have demonstrated the formation of the ultra-wide transmission bands over the suppressed PBGs in a whole range of possible filling factors. The TBs obtained demonstrate a substantial bandwidth (> 200 nm) and a negligible number of ripples within the bands.

In order to fine tune the wavelength position, number and width of the output transmitting or reflecting bands, thermal oxidation of the grooved Si structures was exploited. Based on the generated map of TBs the PhC filter with ultra-wide TB characteristics have been successfully fabricated and characterized. The TB obtained exhibit a high transmission of 92-96% and a substantial bandwidth 1800nm with negligible number of ripples on the top.

The effects demonstrated have practical applications in integrated Silicon microphotonics. It suggests that fabricating interference filters with almost 100% transmission over a selected wide range of the infrared spectrum is practical. Also, we note that the approach suggested can be applied to the design of any micro- and nanostructured semiconductor or dielectric material for application across the entire electromagnetic range.

3.8 References


Chapter 4.

**Micro-cavity Photonic Crystals**

### 4.1 Introduction

Modern Si fabrication technology has advanced remarkably over the last decade demonstrating an unprecedented level of photonics integration [1]. The development of the integrated compact multi-channel filters for different applications, such as, communication systems [2-4], multifunctional sensing [5, 6] and microwave antennas [7] has been important and active area of research in this field. The required characteristics are the high quality factor ($Q$), high selectivity (the ability to separate two adjacent channels), high out-of-band rejection in order to guarantee a low cross talk between channels, low power and possibly low insertion. Moreover, the filter capability of low-power and low-loss tuning of channel properties significantly advances device functionalities for the applications where the reconfiguration is required. In this regard, resonance based devices, such as microring resonators [8, 9], travelling-wave resonators [10] and photonic crystal micro-cavity resonators [11], are the most promising solutions. In this Chapter, we will focus on micro-cavity PhC systems due to their significant advantages over other types of resonators, in terms of device simplicity, ease of integration on Si chip, and power consumption. The main objective of this project was the technological realization and experimental demonstration of an integratable solution for the Si-based band-pass filters with ultra-wide continuous tuning capability. The design of a fine-tunable passband filter proposed in this Chapter is based on a one-dimensional Si photonic crystal technology. It requires realization and tuning of the optical defects within the periodical structure by infiltrating it with liquid crystal, thus transforming PhC mirror into a high efficiency passband filter. An LC is one of the most attractive tuning materials for Si based integrated
Section 4.3 presents theoretical and experimental demonstration of integrated optical narrow-band filters based on single-cavity 1D Silicon PhC. Using an example of the nematic LC E7, with $\Delta n=0.2$, a significant shift of the resonance peak up to 10% at high modulation of reflection/transmission coefficient ($\Delta R$ or $\Delta T) \approx 95\%$) was demonstrated. The precise tuning of the obtained resonance bands was experimentally achieved by either varying the temperature from 10° to 65°C or by application of electric field from 0 V to 15 V. Using the gap map approach as a core engineering tool allows prediction of the formation of transmission bands within the Stop Bands, i.e. photonic band gaps, and, thus, effectively determine the exact optimal design parameters of the filter device.

In Section 4.4 the continuous fine-tuning capability of a LC single micro-cavity is extended to a system of individually tunable, coupled multi-cavities. Application of an electric field to each cavity individually, and its continuous selective variation across all cavities allows problems due to the strong coupling between channels to be overcome. Using an example of a coupled, triple-cavity, PhC filter, operated using the first SBs, we have developed a simple model for easier manipulation of the LC within individual cavities, enabling independent fine tuning of each channel in the overall system. We note that the model suggested can be extended to a higher number of coupled cavities (defects) and, therefore, to a higher number of resonances, with an improved $Q$ value. To the best of our knowledge, there have been no reports in the literature on addressing this problem using electro-tuning for the individual channels in a multi-channel system that is compatible with CMOS (Complementary Metal Oxide Semiconductor) technology.

4.2 Basic Concept: Modelling of 1D micro-cavity Photonic Crystals

A free-space, microstructured grooved Si structure, with quarter-wavelength “Si-air” layers of optical thicknesses

$$d_{Si} \cdot n_{Si} = d_{Si} \cdot n_{air} = m \cdot \frac{\lambda_m}{4}$$  \hspace{1cm} (4.1)
is considered here as a model for an ordinary 1D PhC mirror, where $d_{Si}$, $n_{Si}$ and $d_{air}$, $n_{air}$ are the geometrical thickness and refractive index of Si and air layers, accordingly and $m$ is the order of the SBs. The refractive indexes of Si and air in NIR and MIR are taken from Ref.[12]. As the optical contrast of the PhC, $n_{Si}/n_{air}$, is sufficiently high, only a small number of periods is required to obtain a SB with a reflection, $R$, of greater than 0.99. Let us consider an example of 1D PhC with the number of periods $N=7.5$ and the lattice period $a=d_{Si}+d_{air}$ (Figure 4-1(a)). The optical spectra of this simple structure can be calculated using the Transfer Matrix Method [13]. For all spectral simulations in this Chapter, the optical characteristics are presented in unitless dimensions of normalized frequency ($NF=a/\lambda$) and/or normalized wavelength ($NW=\lambda/a$) and, therefore, can be applied to a wide range of filter sizes and range of operation. For the considered example structure with filling fraction value $f_{Si}=d_{Si}/a=0.243$, the $6^{th}$ order, $m=6$, SB is centred at the normalized wavelength $NW=0.29$ or normalized frequency $NF=3.45$ (Figure 4-1(b)).

The single/coupled resonators induced transparency around the operational wavelength $\lambda_m$, occurs when optical or geometrical defects (micro-cavities) are introduced into a perfect periodical structure [14, 15] (Figure 4-1(c, e)). Formation of a microcavity resonator requires a doubling of the optical thickness of certain periods in 1D PhC

$$n_{cav}^{(i)} \cdot d_{cav}^{(i)} = m \cdot \frac{\lambda_m}{2},$$

(4.2)

where $n_{cav}^{(i)}$ and $d_{cav}^{(i)}$ are the refractive index and the geometrical thickness of the introduced defect (cavity), accordingly, and $i$ is the number of the cavity, thus transforming the broadband mirror into the narrow passband filter. This type of microcavity 1D Photonic Crystals feature Fabry-Perot-style resonators (an optical resonator in which feedback is accomplished using two mirrors, e.g. "Si-cavity-Si") with ultra-high reflectance mirror technology [16]. This can be achieved, for example, by infiltration of the groove with a filler of a suitable refractive index. TMM calculations, performed for the single-cavity PhC structure with 7.5 period, after infiltration of its central groove with an example fillers of refractive indexes $n_{cav}=2$ and $n_{cav}=1.5$ are shown in Figure 4-1(d). The realized resonance peak is centered at $NW=0.289$ ($NF=3.46$) for the $n_{cav}=2$ (black line) and blue shifted to $NW=0.286$ ($NF=3.50$) for $n_{cav}=1.5$ (green line). The reflection spectra of "Si-cavity-Si" Fabry-Perot resonators (FPRs) are plotted in Figure 78.
4-1(d) for \( n \) value of cavity being 1.5 (dashed green line) and 2 (dashed black line) along with \( R \) spectra for single-cavity PhC with 7.5 periods. The \( Q \) of a single-cavity PhC of 7.5 periods is significantly higher, \( Q=15000 \), in comparison to the elementary single 1.5- period (\( N=1.5 \)) FPR for which \( Q \) is only 334.

**Figure 4-1**: Schematic fragments of (a) defect-free 1D PhC and 1D PhCs with (c) single and (e) triple optical defects. (b, d, f) The TMM simulated reflection spectra for the sixth order SB are demonstrated in normalized wavelength units \( NW=\lambda/a \) ((b) lower scale) and normalized frequency \( NF=a/\lambda \) ((b) upper scale). The value of filling fraction is 0.243 and the refractive index of defect is \( n_{cav}^{(1)}=1.5 \) (light green line) or \( n_{cav}^{(2)}=2 \) (black line). \( R \) spectra of the single 1.5 periods FPRs are also shown for comparison (dashed lines).
Similar technique is used for the realization of the multiple-coupled defects (cavities) within the defect-free PhC. From an optical point of view, increasing of the number of coupled cavities results in a mode-splitting effect, i.e. in increase of the number of resonance peaks realized within the SBs and the proportional increase of the $Q$ comparing to the single FPR. In Figure 4-1(e) we demonstrate an example of the triple-optical defect structure with refractive indexes $n_{cav}^{(1)}=n_{cav}^{(2)}=n_{cav}^{(3)}$, realized in a defect-free PhC. The resonance peaks of PhCs with a single cavity have split into three-coupled resonances. The central resonance has retained its wavelength of operation, while the other resonances are separated from the central peak by a fixed resonance-spacing, $\lambda_s$, or by a free spectral range (FSR). For the considered example of a triple-cavity the $Q$ was increased in 3 times, comparing to the $Q$ of a single 1.5-period FPR.

4.3 Single cavity Photonic Crystal: a Fabry-Perot resonator

4.3.1 Gap Map design of Fabry-Perot resonators

4.3.1.1 "Si-air-Si" Fabry-Perot Resonator

In order to draw the map of SBs for 1.5-period PhC (FPR), a set of $R$ spectra (~100 in total) are calculated for filling fraction, $f_{Si}$, varied from 0 to 1 with step of 0.01, assuming that the parameter $\alpha=d_{air}+d_{Si}$ is constant. The obtained values of the reflection coefficient, $R$, are cut off using the criterion $[17, 18] R_{cut}^R>0.85$, while the rest of the values are plotted on the graph versus normalized frequency, $NF$, as shown in Figure 4-2. The lower than usual value of cut off criterion for SBs ($R_{cut}^R=0.85$) for selection of data for gap map formation is chosen for clearer presentation (see Chapter 2 for details).

As shown in Figure 4-2(a), the obtained SBs are relatively wide, that is due to the high optical contrast and the low value of $R_{cut}$. Then the set of calculated $T$ (or $R$) spectra is filtered using another cut off criterion, namely $T_{cut}^T>0.99$. From the obtained data the map of transmission bands (or pass-bands) is plotted on the obtained above map of SBs (see Chapter 3). This is used for more clear demonstration of the location of transmission bands with respect to the SBs depending on $f_{Si}$. Figure 4-2(a) shows the SBs surrounded by the transmission bands. In TB regions the resonance modes with large signal modulation ($\Delta R=0.95$) as well as low signal modulation are included. The second y-axis, from the right side of the plot shown in Figure 4-2(a), presents the filling fraction for air, $f_{air}$, as a part occupied by air relatively to $\alpha$ value, i.e. $f_{air}=d_{air}/(d_{air}+d_{Si})$. 

80
Figure 4-2: (a) Map of stop-bands (shown by red contour with symbolic numeration) with $R>0.85$ and regions of transparency (black contour) with $T>0.99$ for 1.5-period PhC or FPR (shown in insertion). The incoming and outgoing media are air, $n_{Si}=3.42$, and the incidence of light is normal. (b) The $R$ spectrum for $f_{Si}=0.11$ with few largely-modulated resonance peaks between SBs 1a-1b, 2c-2d and 2d-2e. (c) Spectrum $R$ for $f_{Si}=0.4$ demonstrated the absence of narrow resonance peak between SBs 1a-2a, 3b-4b.

Since the resonance peaks in 1D PhC are characterised by a sharp change in transmission (from $-0$ to $-1$) in vicinity of the resonance peak, as a consequence the TB region must be surrounded by two SBs on the GM. Let us consider the structure with the filling fraction $f_{Si} = 0.11$, for example. For this value we draw the horizontal line, which intersects the SB regions as well as TBs. For convenience we numerate the SBs
in order as shown in Figure 4-2(a). It is seen in Figure 4-2(a), that in the region of $NF=0.6$ there is a TB region, which is surrounded by SBs 1a and 1b, while in spectrum $R$, depicted in Figure 4-2(b), the resonance peak is observed at $NF=0.6$. We can also see the presence of resonance peaks with large modulation in the regions $NF=1.7$ and $NF=2.2$, which are predicted from the map between SBs 1b-1c, 2c-2d and 2d-2e for the corresponding values of $f_{Si}$.

Let us now concentrate more precisely on what is observed between SBs 1a and 2a, for example, for $f_{Si}=0.4$ (Figure 4-2(c)). We can see that the transmission peaks observed between these stop-bands are considerably wide. Similar result is obtained for the other values of filling fractions, $f_{Si}$, for transmission bands located between SBs 2a-3a, 1a-2b, 2b-3c and others. Therefore, for considered type of FPR the formation of resonance peaks with large signal modulation can occur in the region of $f_{Si} \sim 0.2$ and below. This rule is related to the fact that for obtaining the total constructive interference for transmission a substantial part of low-refractive index component in a structure is necessary.

4.3.1.2 “Si-LC-Si” Fabry-Perot Resonator

Taking into account the analysis and conclusions made in the previous Section, let us now investigate a 1.5-period FPR, in which the compound with refractive index birefringence (that can be changed by the external forces) will replace the air in the cavity (Figure 4-1(b)). For this purpose we can use the nematic LC E7 with extreme values of the refractive indexes, $n_{LC}=n_{cav}$ equal to 1.49 and 1.69 (see Chapter 2 for details). We calculate the set of $R$ and $T$ spectra and draw the GMs of SBs and TBs for two values of $n_{LC}$ in the resonator cavity (Figure 4-3(a)).

Two types of SBs with defect cavity modes corresponding to $n_{LC}=1.49$ and 1.69 can be seen in Figure 4-3. These SBs are narrower than SBs demonstrated above in Figure 4-2(a) due to the lower optical contrast (in ~1.4 times). From Figure 4-3(a) in the region of $f_{Si}=0.06$ one can observe the intersection of SBs with transmission bands, in vicinity of values $NF=1$, 1.2 and 1.6, for example. More clearly this can be seen on spectra shown in Figure 4-3(b).
Figure 4-3: (a) The map of stop-bands (oval-like figures) and transmission bands (lines) for 1.5-period PhC (FPR) based on 3-layers model "Si-LC-Si" with two values of $n_{LC}=n_1=1.49$ (red contours for SBs and pink lines for TBs) and $n_{LC}=n_2=1.69$ (black contours for SBs and grey lines for TBs). $R_{cutoff}=0.85$, $T_{cutoff}=0.99$. (b) Spectrum $R$ calculated for $f_{Si}=0.06$ and demonstrating the cut off line of $R$ values, used for drawing of SBs map. (c) Fine tuning of peak positions and stop-bands with variation of $n_{LC}$ from 1.49 to 1.69. Relative peak shift $\Delta N F/N F=0.14/1.33=10.5\%$.

The presented spectra demonstrate that the variation of $n$ by 0.2 in resonator cavity leads to the shift of the resonance peak from 1.40 to 1.26 $N F$ resulting in a relative shift value, $\Delta N F/N F = 0.14/1.33 = 10.5\%$. The width of the SB in this diapason is $\sim 0.2 N F$, as well as SB shifts by approximately the half of its width during the tuning. The LC molecules can be oriented in such way, that their refractive index possesses not only the extreme values ($n_o$ and $n_e$), but also some intermediate values. Figure 4-3(c) is depicted the spectra for these intermediate values of $n_{LC}$ that demonstrate the possibility of fine tuning of resonance peaks and stop-bands position.
Thus, using TMM, the reflection spectra of FPR (or 1.5-period PhC) based on structures "Si-air" and "Si-LC" can be calculated. The filtering of these spectra using two criteria for maximum and minimum values of the reflection coefficient provides the set of data for drawing the maps of stop-bands and transmission bands. The resonance bands with large modulation of $R$ values ($\Delta R \approx 0.95$) are located between the certain stop-bands regions. By means of this approach, the range of optimal filing fractions of FPR can be established in the range of $f$ values from 0.05 to 0.4 for achieving a significant shift of SBs and the resonance peaks up to 10% using LC birefringence of $\Delta n=0.2$ with $R$ modulation up to 0.95.

4.3.1.3 *Photonic Crystal with "optical" defect*

To obtain a well pronounced resonance peak, it is necessary to increase at least twice the optical thickness of one of the component in the centre of PhC structure (Figure 4-1(a)). This can be achieved by increasing the geometrical width of the structure (Figure 4-1(c)) or by replacing the air gap ($n=1$) in the centre of structure by a compound with refractive index $n = 2$ (Figure 4-1(d)). If it is not possible to use a compound with $n = 2$, but with smaller refractive index, for example with $n = 1.49$, the resonance peak still appears, but not in the centre of SB. Although, the peak width (quality factor) and the amplitude of signal modulation for this resonance peak are nearly the same as the calculated values for an ideal resonator (at $n = 2$). For the formation of the corresponding defect typically the first stop-band is used. In this Section the investigation of the possibility of using the resonance peaks, formed in SBs of high order, is performed with GM approach.

Let us consider the FPR based on 3-period PhC with "optical" defect. We calculate the gap map for PhC with three periods and draw the map for PhC with central air gap infiltrated by LC, i.e. with refractive index of defect $n_{\text{def}}=1.49$ (Figure 4-4). The gap map demonstrates, as expected [18], that the infiltration of LC into one central groove changes $n$ value from 1 to 1.49, increasing the optical width of this groove and, therefore, results in the formation of the defect mode region by splitting of SBs of any order. For example, the horizontal line on the map, corresponding to $f_{\text{Si}}=0.15$, intersects the SBs and defect bands in the regions of $NF=0.41$, 0.72 and 1.54. For these $NF$ values, very pronounced resonance peaks are observed in spectrum $R$ shown in Figure 4-5(a). Similar appearance of the defect modes is also depicted for $f_{\text{Si}}=0.4$ and 0.6, for
example, as demonstrated in Figure 4-5(b) and Figure 4-5(c) for $f_{Si}=0.4$ and 0.6 as an example.

![Graph](image_url)

*Figure 4-4: (a) The map of SBs for 3-period PhC "Si-air" (black contour) and 3-period PhC "Si-air" with LC "optical" defect (red contour) with $n_{LC}=1.49$*

These examples demonstrate a possibility to cover with resonance peaks the entire range of $NF$ values for PhC resonator of the above mentioned type with using the first stop-band as well as the SBs of high order. During the fabrication of such FPR (or PhCs with optical defect), there can be certain advantage in retaining the same thickness of Si walls and air gap. At the same time in case of PhC with a resonator where a geometrical defect is used, it is necessary to control additionally the size of the resonator cavity.

The map of the transmission bands which are located between the stop-bands is depicted in Figure 4-6. Careful examination of the TBs for this type of resonator shows that it is impossible to generate the resonance peaks with high signal modulation between the stop-bands for any values of $f_{Si}$ (Figure 4-6).
Figure 4-5: $R$ spectra for $f_{Si}=0.15$ (b), 0.4 (c) and 0.6 (d) (see GM in Figure 4-4).

Figure 4-6: The map of SBs for 3-period PhC "Si-LC" with $n_{LC}=1.49$ (red contour) and map of TBs (black lines).
Figure 4-7: (a) The map of stop-bands ($R_{\text{cutoff}}=0.85$) for 3-period PhC "Si-LC" (see insertion) with tunable LC optical defect at $n_{\text{LC}}=1.49$ (red contours) and 1.69 (black contours). (b) Reflection spectra, $R$ for $f_S=0.05$ with $n_{\text{LC}}=1.49$ (red line) and 1.69 (black line); (c) the extended transmission spectra, $T$, with relative peak shift of $\Delta NF/NF = 9.7\%$ for SB 1c.
Next, we investigate how the PBG map will look like when the refractive index of LC defect is replaced by the value of $n_{LC} = 1.69$ (instead of $n_{LC} = 1.49$ used in the previous case). As can be seen from Figure 4-7(a), the first stop-band as well as SBs of high order have changed insignificantly by this replacement of $n$, as expected, since the optical contrast of PhC was not significantly changed. The major changes are observed in the regions of the defect modes, namely, the smaller the $f_{Si}$ values, the larger variations are. For example, in SB obtained at $f_{Si} \sim 0.1$ and $NF=0.6-1.0$ for the modelled transformation at given value of $\Delta n=0.2$, two defect modes with a consequent band shift may appear instead of one mode. This can be explained by an increase of the optical width of the cavity. As the purpose of this Section is to consider how the maximal shift of the resonance peaks can be achieved, we have to analyse the following points. What values of $f_{Si}$ must be selected to obtain the resonance peaks in the limited range of SB width? To make the solution easier, the $f_{Si}$ values must be in the range where SB is the widest. In Figure 4-7(a) this region of SB corresponds to $f_{Si}<0.5$. We note that this range of $f_{Si}$ is larger than in case of “Si-air” structure (see Figure 4-2(a)) where $f_{Si}<0.2$.

The regions of defect modes must also demonstrate the maximal shift and at the same time the resonance peak with minimal $n=1.49$ located near the blue edge of SB, since when the value of $n$ increases to 1.69, the resonance peak should not leave a selected stop-band. As can be seen from Figure 4-7 (a), the width of SBs 1a, 1b, 1c, and 1d, for example for $f_{Si}=0.05$, is large enough to accommodate both resonance peaks. Based on these conditions, it is more preferable to select PhC with $f_{Si}=0.05$, for which the spectrum $R$ is depicted in Figure 4-7(b). Figure 4-7(b) shows that the maximal shift of the resonance peak is provided by SBs 1c. Figure 4-7(c) demonstrates the extended transmission spectra, $T$, for SB 1c. The resonance peak is shifted from 1.27 to 1.4 $NF$ correspondent to $\Delta NF/NF = 9.7 \%$.

The obtained dependencies enable us to design the tunable filters for selection of the required transmission band. For this design it is necessary to select the operational range of frequencies (or wavelengths), to determine the lattice constant, $a$, a refractive index of a filler and the filling fraction of Si, $f_{Si}$. 

88
4.3.2 Experimental: Fabrication and Optical Characterization

The FBRs with optimal design parameters were fabricated using optical lithography and anisotropic chemical etching of (110)Si [19] as well as DRIE process of (100)Si [20]. For fabrication of the passive FPRs the conventional Si wafers were used while tunable LC-FPR devices were formed on (110) Si-on-insulator (SOI) wafers. The thickness of the Si device layer and the Buried Oxide (BOX) layer were 20 µm and 2 µm, respectively. Thermally grown Silicon dioxide was used as a mask when etching the wafers. The choice of 20 µm for the depth, in particular, was dictated by the minimum size of the IR microscope aperture used for optical characterization, in conjunction with an FTIR, FTS 6000 spectrometer [21] (Chapter 2). The example of Silicon resonator, fabricated on (110)Si is depicted in Figure 4-8. The SEM investigation has demonstrated quite smooth (practically mirror-like) Si sidewalls of the structure fabricated by anisotropic chemical etching (Figure 4-8(b)). At the same time, the roughness of Si sidewalls, obtained after DRIE, is quite substantial (see Section 4.3.2, Figure 4-13(f)). The cavity was infiltrated with commercial LC E7 (Merck) [22] using a specially designed reservoir and the channels shown in Figure 4-8(a).

![Figure 4-8: SEM images of air-resonator, fabricated on SOI platform, using (110)Si, with (a) reservoir for LC infiltration and b) the cross-section of the resonator edge. Depth of Si-walls is \( h_{Si} = 20 \mu m \).](image)

Optical characterisation was performed with a polarized FTIR microspectrometer in reflection, \( R \), and transmission, \( T \), modes in the wavenumbers range of \( \nu = 650-6500 \text{cm}^{-1} (\lambda = 1.5-15 \mu m) \). For polarized infrared measurements, the electric vector of the incident light is aligned with the Si grooves for \( E \)-polarized light, while for \( H \)-polarized light the electric vector is aligned along the depth direction of the grooves.
as shown in Figure 4-9. For characterization of the structure in the Near Infrared (NIR) range $\lambda=0.9\text{-}1.7\ \mu m$ the optical fiber-coupling set-up based on an OSA was used. The setup was developed for the purpose of polarized transmission measurements in the NIR range. The characteristic vibrational bands of the liquid crystal were also analysed, together with the interference bands of high reflection, the Stop Bands, and the resonant transmission peaks. Note that all the experimental spectra ($R$ and $T$) are presented in this Section in arbitrary, or normalized, units in order to clearly compare the results. Normalization of the data was necessary due, in particular, to a shading effect [21] of the focused light beam onto the Si wall of the resonator, integrated onto the chip, during infrared measurements (see Chapter 2 for details).

Figure 4-9: Schematic presentation of Fabry-Pérot resonator, consisting of two Si walls separated by (a) a gap and infiltrated with liquid crystal molecules with different alignment: (b) vertical planar, (c) horizontal planar, (d) isotropic, (e) homeotropic and (f) horizontal planar with air voids.
The obtained experimental spectra were fitted using the chosen model for the three-layer system ("Si-air-Si" or "Si-LC-Si"), which allows us to obtain the precise values of the thicknesses $d_{Si}$ and $d_{cav}$ as well as $n_{LC}$, served as fitting parameters. Both thickness values, obtained from the fitting coincide well with the results estimated from SEM images. The used nematic LC E7 is a dispersive material demonstrating three absorption bands in MIR at 1497 cm$^{-1}$, 1606 cm$^{-1}$ and 2226 cm$^{-1}$. The dispersion formula for the ordinary and extraordinary refractive indexes can be described as:

$$n_o = 1.4990 + 0.0072\lambda^2 + 0.0003\lambda^4$$

$$n_e = 1.6933 + 0.0078\lambda^2 + 0.00028\lambda^4$$

The variations of $n_{LC}$ values with wavelength are not significant and, hence, were not considered in the spectra simulations.

4.3.2.1 Fabry-Perot resonator fabricated by anisotropic etching of (110)Si

The polarized reflection spectra $R$ of the resonator, fabricated by anisotropic etching of (110)Si, are discussed in this Section. The experimental, $E$-polarized reflection spectra of the air and LC resonators are shown in Figure 4-10(a). This figure depicts the characteristic interference bands spread uniformly throughout the entire range of spectra from 650 to 6500 cm$^{-1}$ (15-1.5 μm). The fitting of the registered spectra was performed until the best fitting was achieved at certain fitting parameters $d_{Si}$ and $d_{cav}$. The spectrum calculated with the best fitting parameters ($d_{Si}$=1.2 μm and $d_{cav}$=3.4 μm) is shown in Figure 4-10(b) for $n_{cav}$=1. As can be seen from Figure 4-10(b) the calculated spectrum shows four characteristic resonance peaks, which are also observed in the experimental spectrum with some degradation of peak quality.
Figure 4-10: The (a) experimental and (b) calculated reflection spectra for air (dashed line) and LC (solid line) resonators. For spectrum, shown in (b), $n_{\text{air}}=1$ (dashed line) and $n_{\text{LC}}=1.72$ (solid line) for $d_{\text{Si}}=1.2 \ \mu\text{m}$ and $d_{\text{cav}}=3.4 \mu\text{m}$. The height of Si wall is $h_{\text{Si}}=50 \mu\text{m}$.

The latter is demonstrated as a broadening of the resonance peaks as well as decrease of the peak’s amplitude. This degradation could be caused by few factors such as the focused light beam of the FTIR microscope, shading effect, unevenness of the Si walls and others. Nevertheless, the position of all experimental SB peaks is in a good agreement with calculated spectrum, which confirmed a good quality of the Si sidewalls and their correspondence to the desired geometrical parameters. The infiltration of LC into the cavity results in substantial blue-shift of nearly all of the interference bands (IBs), which reflects the increase in the refractive index of the resonator cavity. Moreover, the shape of the resonance peaks becomes more distinct.
Figure 4-11: The (a) experimental and (b) calculated reflection spectra for LC-resonator for E-(solid line) and H-polarization (dashed line). Calculated spectra with $n_{LC} = 1.72$ (solid line) and $n_{LC} = 1.53$ (dashed line), $d_{Si} = 1.2\mu m$ and $d_{cav} = 3.4\mu m$.

As is well known a decrease in the optical contrast at the interface of two phases diminishes the effect of light scattering, which can influence the peak quality and thereby explains some improvement in the resonance peaks quality. The fitting of the reflection spectra $R$ for LC-resonator with the same parameters $d_{Si}$ and $d_{cav}$, but at variation of $n_{cav}=n_{LC}$ in the range from 1.3 to 1.8, leads to a reflection spectrum $R$ for E-polarization, shown in Figure 4-10(b) (solid line) at $n_{LC} = 1.53$. Quite good agreement is observed again between calculated and experimental spectra in Figure 4-10. A similar approach was used for fitting the $R$ spectra of the LC-resonator for H-polarization, and both spectra (for E- and H- polarizations) are shown in Figure 4-11. Figure 4-11 reveals that the $R$ spectrum for E-polarization for three lowest SBs is blue-shifted with respect to that for H-polarization. Apart from this, the resonance peaks are observed on Figure 4-11 in maxima of IBs at $\sim 3300$ cm$^{-1}$ and at $\sim 4200$ cm$^{-1}$ as was predicted by GMs in Section 4.3.1.
As was already shown for the $E$-spectrum, the fitting of $H$-spectrum demonstrates a very good convergence between experimental and calculated spectra at $n_{LC}=1.53$. From the fitting we receive practically the same value of birefringence of LC E7 which is $\Delta n=0.19$ comparing to the literature [23], but slightly different values for the ordinary and extraordinary refractive indexes: $n_o=1.53$ and $n_e=1.72$. At the same time, the high value of $\Delta n$ is also confirmed by the appearance of the characteristic vibrational bands of LC E7 [24] at 1497, 1602 and 2222 cm$^{-1}$, which are observed in the $E$-spectrum and almost absent in the $H$-spectrum. Therefore, one can conclude that the spontaneous planar orientation of the LC director along the channel has occurred, which corresponds to the schematic, presented in Figure 4-9(c). The experimental $R$ spectra versus wavelengths (the same ones as presented in Figure 4-11(a) vs. wavenumbers) are presented in Figure 4-12(a) with extension to the NIR range 1.5–3 µm. A good correspondence between the positions of $R$ bands and the resonance peaks is observed.

**Figure 4-12:** The (a) experimental and (b) calculated reflection spectra in NIR range vs. wavelengths (from Figure 4-10).
in the regions of 1.7-1.8 and 2.2-2.35 μm, which is in agreement with the calculated data shown in Figure 4-12(b).

Thus, the resonator with $d_{\text{cav}}=3.4$ μm demonstrates quite promising characteristics as follows from simulations. If it is an LC-resonator, then, $\lambda_0=(2\cdot1.6)\cdot d_{\text{cav}}=11\mu$m and $d_{\text{Si}}=11/(3.42\cdot4)=0.8\mu$m. During fabrication we have received a resonator with $d_{\text{Si}}=1.2$ μm, which is quite close to the calculated value. We can, therefore, conclude that the LC-resonator with a working wavelength of 11 μm (or ~910 cm$^{-1}$) is fabricated. The resonance peak of this FPR is seen in experimental and in calculated reflection spectra (Figure 4-11). In addition to that, the corresponding resonance peaks of 2$^{\text{nd}}$, 3$^{\text{rd}}$, 4$^{\text{th}}$ and 5$^{\text{th}}$ SBs are perfectly depicted in the calculated as well as in experimental spectra of air and LC resonators (see Figure 4-10...Figure 4-12).

4.3.2.2 Fabry-Perot resonator fabricated on (100)Si by deep reactive ion etching

Let us now investigate a non-ideal resonator with non-optimal calculated parameters. In contrast to the previously described FPR, this resonator is fabricated on (100)Si by DRIE process. In this case, if the depth of the etching is relatively large, quite significant roughness of the Si sidewalls is observed (see Figure 4-13(e, f)), which may strongly influence the quality of the experimentally registered spectra. Another distinct feature of this resonator is the smaller depth (or height, $h$) of its Si walls ($h_{\text{Si}}=20$ μm). The decrease in the height of the Si walls results in a decrease of the aperture of the incident light beam, which in turn leads to reduction of the signal-to-noise ratio during FTIR measurements.

The experimental and calculated reflection spectra for air and LC resonators are presented in Figure 4-13(a-d). The interference bands in spectrum $R$ are deformed and demonstrate the reduced amplitude modulation and so only the part of the spectral range below 4000 cm$^{-1}$ is shown. The fitting of this reduced range of spectra (650 – 4000 cm$^{-1}$) for the air resonator (see Figure 4-13(a)) yields the following parameters of the resonator: $d_{\text{Si}}=2.6$ μm and $d_{\text{cav}}=5.4$ μm. Therefore, if we use this resonator as a resonator calculated for utilisation with LC, then it’s working wavelength (the position of the first resonance peak) will correspond to $\lambda_0=2\cdot1.6\cdot d_{\text{cav}}=17.3$ μm and the thickness of the Si walls to $d_{\text{Si}}=17.3/(3.42\cdot4)=1.26$ μm.
Figure 4-13: The (a, b) experimental reflection H-spectra of empty (dashed line) and LC (solid line) resonator vs. (a, c) wavenumber and (b, d) wavelength. (c, d) Calculated spectra with \( n=1 \) (dashed line) and \( n_{LC}=1.53 \) (solid line). SEM images of the resonator: (e) the top view and (g) a sidewall roughness, obtained after DRIE of (100)Si, \( h_{Si}=20 \mu m \).

Thus, according to the calculations, the obtained resonator does not have optimal parameters and, as a result, the position and the quality of the resonance peaks will be different. Nonetheless, the characteristic peaks (dashed lines in wavenumber (Figure 4-13(a, c)) and in wavelength (Figure 4-13(b, d)) presentations) at \( \sim 1300 \text{ cm}^{-1} \) (7.7 \( \mu m \)) and at \( \sim 2500 \text{ cm}^{-1} \) (4 \( \mu m \)) are well identified during the fitting as resonance peaks in
the reflection spectrum of the air resonator. After the infiltration of the air cavity with LC, the $n_{\text{cav}}$ changes and this leads to change in the experimental and calculated spectra $R$, denoted by solid lines in Figure 4-13(a, b) and Figure 4-13(c, d), respectively. Performing the fitting with known parameters $d_{\text{Si}}=2.6 \, \mu\text{m}$ and $d_{\text{cav}}=5.4 \, \mu\text{m}$, we find the value of $n_{\text{cav}}=1.53$. This value of $n_{\text{LC}}$ provides the shift of spectral patterns in such a way that at the frequency of $\sim 900 \, \text{cm}^{-1}$ (11 \, \mu\text{m}) the empty resonator $R$ has high values, while for LC-cavity the values of $R$ are low. A reverse situation is observed at frequency of $\sim 2500 \, \text{cm}^{-1}$ (4 \, \mu\text{m}) where for the empty resonator the low $R$ values are obtained, while for the LC-cavity the $R$ values are high. Therefore, it was shown that an LC resonator can be designed even with non-optimal parameters and despite this it can possesses relatively good optical characteristics close enough to the calculated values of an ideal resonator. It was also shown that the roughness of Si sidewalls impairs the quality of the resonator fabricated on Si using the DRIE technique.

4.3.3 Ultra-wide tuning of resonance modes

4.3.3.1 Thermo-tunable single channel devices

The tunable LC resonator was fabricated on (110)Si by anisotropic etching, in which the tuning of optical properties was obtained due to the reorientation of LC molecules (or LC director) as was predicted by GM in Section 4.3.1. Initially, the reflection spectrum, $R$ of an air resonator was measured and its parameters were determined, using a fitting procedure as described in previous Sections. The air resonator parameters were chosen close to the ideal ones, as described in Section 4.3.2; the parameters obtained during the fitting of the reflection spectra are: $d_{\text{Si}}=1.2 \, \mu\text{m}$ and $d_{\text{cav}}=3.6 \, \mu\text{m}$. 

97
Figure 4-14: (a, c) The experimental reflection spectra of LC resonator, demonstrated the effect of thermo-tuning, namely the transition from LC mesophase at 20 °C (dashed line for H- and thin line for E-polarization) to the isotropic phase at 65 °C (thick line). (b, d) Calculated spectra with $n_{LC} = 1.67$ (thin line), $n_{LC} = 1.54$ (thick line) and $n_{LC} = 1.5$ (dashed line). $d_{cav} = 3.6 \, \mu m$, $d_{Si} = 1.2 \, \mu m$ and $h_{Si} = 50 \, \mu m$.

Then, the cavity was infiltrated with LC E7 and the reflection spectra were measured at room temperature for E- and H-polarization of the incident light (see Figure 98).
As can be seen from Figure 4-14(a), the spectra $R$ are shifted at different polarizations. The fitting, performed for $R$ spectra (Figure 4-14(b)), enables the value of $n_{LC}$ to be determined from each of these spectra. The $n_{LC}$ value, obtained for $E$-polarization is 1.67, while for $H$-polarization $n_{LC}=1.5$. Moreover, as can be seen from Figure 4-14(a), the characteristic vibrational bands of LC E7 at 1497, 1603 and 2222 cm$^{-1}$ are also present in the spectrum $R$ only for $E$-polarization, which confirmed that LC has a pronounced spontaneous orientation of rod-like molecules along the channel. This type of LC orientation is shown schematically in Figure 4-9(c) and is one of the most common types of alignment, obtained in this work during LC-infiltration into 1D PhCs air channels by capillary effect.

The resonator was heated up to 65°C using a calibrated thermocouple micro-heater and the reflection spectrum was registered again at this temperature (Figure 4-14(a)). The variation of $n_{SR}$ at heating to 65°C is not larger than 0.001 and, therefore, can be neglected in this case. Using the fitting of the registered reflection spectrum, the value of $m_{LC}$ was estimated to be around $n_{LC}=1.54$. Two spectral effects were revealed for $R$ spectrum at $E$-polarization (see the stop-band in Figure 4-14 shown by circle). In particular, the resonance peak, observed at frequency $\sim 5100$ cm$^{-1}$ (at wavelength of 1.94 μm on Figure 4-14(c)), is situated quite close to the maximum of reflection from the heated resonator (thick line). The value of $R=0.25$ a.u. is observed at this resonance peak at room temperature, while at 65°C the maximum of reflection increases up to $R=0.4$ a.u. At the same time, at frequency of $\sim 5300$ cm$^{-1}$ (wavelength 1.94 μm) the reflection is $R=0.41$ a.u. at room temperature, while at heating of LC to 65°C and its transition to isotropic phase (see Figure 4-9(d)) the resonance peak at $\lambda=1.9$ μm with $R=0.19$ a.u. is appeared. Thus, the thermo-optical effect of LC can be used at two wavelengths. With improved fabrication technology of this type of FPRs, the much higher ratio of the reflection values (up to 0.01/0.89) for these two cases can be achieved (Figure 4-14(d)). Unfortunately in this type of experiment it is difficult to return to the original LC orientation after cooling the structure down to room temperature. However, this example demonstrates the principle of tuning the resonator for controlling the relative intensity of the reflected light of certain polarizations. It is also demonstrates the possibility of utilizing the observed optical effects in SB and in resonance peaks of high order.
4.3.3.2 Electrically tunable Fabry-Perot resonator

The electro-tunable LC-FPR was fabricated using optical lithography and anisotropic etching of (110) SOI wafer. A view of the resonator, fabricated on (110) Si, is depicted in Figure 4-15. Si wall-electrodes were connected to the outer pads by attaching thin metal wires to the chip contact areas with conductive silver paste. An AC rectangular pulse train, with various amplitudes between 0.5 V and 15 V, with a pulse duration of \( \tau_p = 1 \) ms and a frequency of \( f_p = 100 \) Hz was used to drive the device [25].

![SEM image of the top view of the FPR fabricated on an SOI wafer.](image)

A best fit to the experimentally measured spectra was performed using using the Transfer Matrix Method [12] was performed. For the empty resonator \((n_{\text{ cav}}=1)\) the fit was performed with a Si wall width of \( d_{\text{Si}} \approx 1 \pm 0.3 \) μm and a cavity width of \( d_{\text{ cav}} \approx 4.0 \pm 0.3 \) μm as fitting parameters, while for the LC FPR, \( n_{\text{ cav}} \) was used as a fitting parameter.

Reflection spectra in \( E \)- and \( H \)-polarization, registered from a 20x20 μm² area of an LC FPR prior to the application of the electric field are shown in Figure 4-16(a). A pronounced shift of the interference bands in the reflection spectra as a result of the change in the polarization of the probe beam from \( E \)- to \( H \)-polarization is observed, confirming the anisotropy of the LC molecules infiltrated into the resonator. In other words, this shift is caused by the alignment of the LC director along some preferred orientation within a Si groove and, therefore, due to the influence of the ordinary, \( n_o \), and extraordinary, \( n_e \), refractive indexes for the appropriate polarization. Similar results are obtained from the same spot when measuring the transmission, \( T \), spectra (Figure 4-16(b)). We note that the transmission spectra are noisier than those taken in reflection,
due to the reduction in the total intensity of the light transmitted through the resonator. Also, the 20% reduction of the $R/T$ signal comparing to the predicted in theory is due to the "shading effect" from the substrate of the fabricated FPR as well as the non-parallel light source used for the measurements (see Section 2.4). Nevertheless, general trends in the behavior of reflection and transmission spectra are clearly seen from a comparison of Figure 4-16(a) and Figure 4-16(b). For both polarizations, the position of the minima in the transmission spectra corresponds to the maxima of the reflection spectra and *vice versa*.

![Figure 4-16: FTIR (a) reflection and (b) transmission spectra of the FP resonator with LC filler for E-(thick line) and H-(thin line) polarizations in the absence of an applied electric field. The resonator parameters are: width of Si walls, $d_{Si}=1 \mu m$, cavity width, $d_{cav}=4 \mu m$.](image)

A fit to the $R$ spectra from the LC FPR results in a value of $n_{cav}=1.57$ for $E$-polarization, and $n_{cav}=1.45$ for $H$-polarization, using known values of $d_{Si}=1 \mu m$ and $d_{cav}=4 \mu m$. The value of $n_{cav}=1.45$ for $H$-polarization obtained appears to be smaller than the value of $n_o=1.49$ from the literature for LC E7 [23]. This discrepancy will be discussed in the following Section. The presence of the LC in the cavity is confirmed by
observation of the absorption band of LC E7 molecules at 2222 cm\(^{-1}\) [24] in the \(R\) (Figure 4-16(a)) as well as in the \(T\) (Figure 4-16(b)) spectra for \(E\)-polarization. We note that for the \(H\)-spectrum, this band is suppressed significantly in comparison to the \(E\)-spectrum. This behavior is typical due to the dichroism of LC molecules. The dominant behavior of the band at 2222 cm\(^{-1}\) for \(E\)-polarized spectra indicates a preferred orientation of the LC director in the \(X\)-direction, along the groove, as shown in Figure 4-9(c).

\[\text{Figure 4-17: Experimental (a) reflection and (c) transmission spectra in } E\text{-polarization in the absence (}0\text{V – thin line) and presence (}10\text{V thick line) of an applied electric field. The spectral shift observed demonstrates the reorientation of LC molecules in the FP-cavity from planar to homeotropic alignment, b) Calculated reflection spectra, obtained from the best fit, for two values of } n_{\text{car}} \text{ shown beside the curves. Resonance peaks are seen at 1800, 2320 and 3400cm}^{-1}, \text{ corresponding to 5.6, 4.2 and 2.9}\mu\text{m.}

Under an applied voltage of 10V, the \(E\)-spectra are blue-shifted, as seen in Figure 4-17(a, c), indicating that the value of \(n_{\text{LC}}\) is reduced in the resonator by the
electric field. The $H$-spectra are practically unchanged by the electric field (not shown). The intensity of the vibrational band of the LC at 2222 cm$^{-1}$ is decreased in the $E$-spectrum at 10V (Figure 4-17(a, c)), indicating that a reorientation of molecules from the initial, planar, alignment to homeotropic alignment has occurred, in accordance with the model presented in Figure 4-9(c, e). The obtained value of $n_{\text{cav}} = 1.45$ (at 10V) appears to be lower in this case than the $n_{\text{cav}} = 1.57$ previously observed at 0V in the $E$-polarized spectrum. In the former case, the orientation of the LC is driven by the electric field and is strongly expected to be homeotropic. In accordance with the schematic shown in Figure 4-9(b), for homeotropic alignment of LC molecules, $n_{\text{cav}}$ must correspond to the refractive index, $n_o$, of LC E7, i.e. to be equal to 1.49. The value of 1.45 obtained from the fitting routine is smaller than 1.49 by 0.04. This deviation is larger than any inaccuracies that one would expect from determining the value of $n$ from the fitting routine with typical deviation of $\Delta n = \pm 0.02$.

As was already noted above, after infiltration of the LC into FPR, the determined value of $n_{\text{cav}}$ was 1.57 for the $E$-spectrum (significantly lower than in the previous Section). This value is close to the expected value of refractive index for a random orientation of the LC molecules $n_{\text{ran}} = 1.56$ [23]. However, dichroism, clearly observed for the 2222 cm$^{-1}$ absorption band, indicated that the initial orientation of LC molecules was planar. In this case, in accordance to literature, $n_e$ must be equal to 1.69 [23], while from the fit of the spectra a significantly smaller value of $n_{\text{LC}} = 1.57$ was obtained. Therefore we conclude from the spectral fitting process that both of the calculated $n$ values ($n_o$ and $n_e$) are smaller than those predicted by the model.

One possible reason for the lower values of $n_{\text{LC}}$ here could be the presence of air voids inside the groove with LC. Indeed, air voids are visible in some SEM images of the LC infiltrated devices. In order to avoid the appearance of air voids, it is better to perform the infiltration of the LC at higher temperatures, typically at the temperature of the isotropic phase. However, in comparison to the previous experiment, the infiltration of the LC was intentionally carried out at room temperature, when the LC E7 is in the nematic phase. An infiltration under these conditions results in a spontaneous planar orientation of the LC director, either along the depth or along the length of the grooves [26]. In the experiment, the degree of infiltration of LC in the groove is normally observed using an optical microscope, allowing the propagation of the LC molecules
along the groove, the $X$ direction in Figure 4-9(c), and the infiltration quality to be assessed.

The results obtained using the Effective Medium Approach (EMA) [27] indicate the possibility of the existence of a volume fraction of air voids in the cavity of $V_{air} = 0.08$, i.e. 8% (Figure 4-9(f)). This could explain the lower values of $n$ obtained from fitting the experimental spectra for both $E$- and $H$- polarizations.

The spectrum registered across the whole infrared range, as well as the spectrum in the region of the vibrational mode at 2222 cm$^{-1}$, reverts to that originally seen at 0 V after the electric field is switched off. Therefore, in this work, we have demonstrated, for the first time, a spontaneous planar orientation of nematic LC molecules on an untreated Si surface, which can be reversed by the removal of the electric field, using voltages up to 10 V. As a result of electrotuning, the FP peaks are shifted reversibly by 128, 168 and 206 cm$^{-1}$, corresponding to relative shifts of $\Delta\lambda/\lambda = 4.2$, 5.2 and 4.8%.

Figure 4-18: Smooth tuning of the position of the resonance peak from 3330 cm$^{-1}$ to 3550 cm$^{-1}$ for $E$- and $H$-polarization (dotted line). The applied voltage is shown in Volts beside each curve.

We also investigated the resonant peak shifts at intermediate applied voltages between 0 V and 10 V, as demonstrated in Figure 4-18 for $E$-polarization in the spectral range from 3000-3800 cm$^{-1}$. The applied voltage of 1.5 V is not enough to cause reorientation of the LC from one state to another. At 2.5 V, which is close to the
threshold voltage of LC E7 (1.5 V), a pronounced shift of the bands is seen. The shift reaches a maximal value at a voltage of 10 V. We note that the position of the resonance peak at 10 V for E-polarization corresponds to the position of this peak at 0 V for H-polarization, as expected from the alignment models demonstrated in Figure 4-9(c, e).

**Figure 4-19:** (a) Experimental and (b) calculated E-polarized spectra of the FP resonator with $d_{Si}=0.6 \mu m$ and $d_{ca}=7.4 \mu m$ without electric field (thin line) and with an electric field generated by an applied voltage of 15 V (thick line). Application of a voltage of 15 V results in a shift of the resonance peaks across the spectral range. The best fit is obtained at $\Delta n_{LC} = 0.17$ ($n_{LC} = 1.51, 0$ V) and ($n_{LC} = 1.34, 15$ V).

A similar experiment was conducted on a different sample with a higher filling fraction of $f_{LC} \approx 0.9$ ($f_{Si} \approx 0.1$). By fitting the experimental spectrum for the empty sample, a value of $d_{Si} = 0.6 \mu m$ was obtained, with a resonator cavity width, $d_{ca} = 7.4 \mu m$ ($f_{Si} = 0.07$). The reflection spectrum, registered for this sample after LC infiltration, demonstrate the shift of the band positions, depending on the polarization of the probe beam, that is, the system exhibits anisotropy. For E-spectrum of $R$ (Figure 4-19(a)), all three characteristic vibrational bands of the LC (at 1497, 1602 and 2222 cm$^{-1}$) have a higher intensity than those in the same spectrum taken using H-polarization (not
shown). This indicates that certain orientation of the LC molecules along the X-axis has occurred (Figure 4-9(c)). Reflection spectra in $E$-polarization, registered after electric field application, are shown in Figure 4-19(a). The applied voltage of 15V results in a blue-shift of the $E$-spectrum, and to a decrease in the intensity of the LC peaks, as demonstrated previously, causing a homeotropic orientation of the LC molecules (Figure 4-9(e)). The results of the best fit to the experimental spectra, using $n_{LC}$ as a fitting parameter and values of $d_{st} = 0.6 \mu m$ and $d_{cv} = 7.4 \mu m$, are presented in Figure 4-19(b). The characteristic FP peaks are seen in the calculated spectrum, which coincide well with the corresponding experimental peaks across the spectral range investigated from 650 to 6500 cm$^{-1}$ (see Figure 4-19(a)). The shifts in the experimental spectrum, obtained after the application of an electric field, are also confirmed in the simulated spectrum. In addition, after the application of voltage of 15 V, the intensity of all three vibrational bands of the LC decreases significantly, confirming the transition of the LC to a homeotropic alignment.

The electro-optical effect observed here can be considered as a reversible, because after the electric field was switched off (0 V) the spectrum returns to its initial state, corresponding to a planar orientation of the LC molecules. The same effect was observed in the first sample, discussed earlier. Figure 4-20 shows intermediate spectra, obtained using a range of applied voltages from 0 V to 15 V, in an extended spectral region from 1480 to 2300 cm$^{-1}$. These spectra demonstrate the possibility of fine tuning of the resonance peaks. This tuning effect is clearly apparent, for example, in the vicinity of $\sim$ 1750 cm$^{-1}$ ($\lambda = 5.7 \mu m$). The reorientation of LC molecules under an applied voltage is also clearly demonstrated by the change in intensity of the 1602 cm$^{-1}$ vibrational band. As noted earlier, the values obtained for the parameter $n_{LC}$ calculated during the fitting routine, are slightly lower than the ordinary and extraordinary refractive indexes of LC E7 from the literature. Note that the values of birefringence of 0.12 and 0.17 are close to the $\Delta n_{LC} = 0.2$ obtained for LC E7 in the mid-IR range [23]. We assume that the lower $n_{LC}$ values obtained here are related to the presence of a small number of voids in the LC, formed during the LC infiltration process.
Figure 4-20: Smooth tuning of the resonance peak from 1700 to 1880 cm$^{-1}$ in the experimental reflection spectra of the FP resonator (from Figure 4-17) with a maximal relative shift of $\Delta\lambda/\lambda = 10\%$.

An electro-tunable LC FPR, based on the principle of changing the optical thickness of the LC resonator, using resonance peaks of high order, has been demonstrated in this investigation. This electro-optical device is based on microstructured Silicon with LC filler. The closest existing analogue to the device suggested is a hybrid photonic crystal microcavity switch, as described in Ref. [28]. In this device, a relative shift in the resonance mode of the order of $(\Delta\lambda/\lambda) = 0.5\%$ in the near infrared range was achieved as a result of the electro-optical effect obtained due to the reorientation of LC E7 in the cavity of a two-dimensional PhC. We would also like to mention Ref. [29], where a shift of the resonance peak of $(\Delta\lambda/\lambda) = 0.5\%$ was reported, due to a variation in the geometrical thickness of the FP air cavity driven by an electric field applied to the second movable mirror. Therefore, the FPR fabricated in this work, fabricated by microstructuring of Si, is significantly better than comparable devices, based on the fact that the resonance peak shift is reached up to 5-10%.
This can be explained by the fact that

i) the resonance peaks in the stop bands of high order were utilized, where a significant shift of the consequent defect mode can be obtained as a result of the change in $\Delta n$ in the electro-optical material used

ii) in comparison with the rough interface in a 2D microcavity, the application of an LC with plane-parallel reflectors provides the most effective distribution of “switchable” molecules with respect to the Si side-walls and the applied electric field.

Investigations of the optical properties of electro-optical devices in the mid-IR range are also technologically important. “Si-LC” composite materials, and switchable elements based on them, are being researched aggressively, due to their transparency in this spectral range and these devices may have application in biochemical sensing, medicine, defense and security [1].

### 4.4 Coupled multi-cavity Photonic Crystals resonators

In Section 4.3 the investigation of FPRs constructed from “Si-air-Si” and “Si-LC-Si” structures demonstrated its effectiveness as a fine tunable filter with a shift of the resonance peak up to $\Delta \lambda / \lambda = 10\%$. This result has demonstrated the largest experimental shift, achieved up to date for the microstructured resonators based on Si, and utilized for molding of light propagated parallel to the substrate. In this Section the continuous fine-tuning capability of the LC single microcavity was exploited to the situation of individually tunable coupled multi-cavities. Application of the voltage to each cavity individually and its continuous random variation in all cavities allows to overcome the problem of strong coupling between channels. Using the example of coupled triple-cavity PhC filter a simple model for easier manipulation of LC within individual cavities have been elaborated, which enables independent fine tuning of each channel in the entire system. Based on the obtained results, prototypes of integrated triple-cavity PhC filters were designed and fabricated on SOI platform. Finally, using a fabricated prototype device as an example, one of the applications of the proposed method, in particular an optimization of the filter to its initially designed operational mode after fabrication process, is demonstrated.
For clarity of presentation of the methodology in this Section, we will focus only on PhC structures with a triple-coupled defect. It should be noted that the suggested model can be extended to a higher number of the coupled cavities (defects) and, thus to a higher number of resonances with improved $Q$ value.

### 4.4.1 Methodology

Although the wide and precise tuning of the resonance peaks in single cavity and double cavity systems, using optical anisotropy of the LC, have been extensively studied in the past years [30-33], only the simultaneous coupled resonances tuning or coupled FSR tuning was demonstrated so far. Indeed, the optical properties of the coupled micro-cavities are strongly dependant on each other, i.e. changing the parameters of one of the coupled cavities directly leads to the change of the optical properties of the others. This coupling effect makes the individual tuning of the resonances almost impossible. Non-trivial solutions for the refractive index variations are needed.

**Figure 4-21:** (a) Schematic view on the variation of the refractive index of LC E7 in the cavity under an applied voltage $V$ (see Section 4.3). (b, c) The controlled variation of the $n_{cav}^{(1)}$, $n_{cav}^{(2)}$, $n_{cav}^{(3)}$ that can be realized in triple-cavity system.
In Figure 4-21(a), using the example of nematic LC E7 (with \( n \) varied in the range 1.49 - 1.69) [22], the fundamental idea of the electro-tuning of the cavity mode is demonstrated schematically based on the results obtained in Section 4.3. Here, it is assumed that the original orientation of the rod-like molecules of nematic LC E7 is along the Si-walls, which ideally results in the refractive index \( n_o = 1.69 \) [23]. Under an applied voltage, \( V = 1.5...15 \) V, the LC molecules reorient in the cavity, which results in decrease of the effective refractive index of the LC. Obviously, this process enables to achieve a precise, continuous tuning of the cavity resonance peaks in a wide range of wavelengths [20]. By increasing the number of the coupled cavities, similar continuous tuning can be achieved for all multi-resonances simultaneously.

Let us consider the case when the electric field is applied to each micro-cavity individually. Then, by increasing or decreasing the applied voltage by \( \Delta V \) in the various cavities, different variations of the LC refractive indexes can be realized, \( n^{(i)}_{cav} = n_0 \pm \Delta n \). For the considered example of triple-cavity PhC, the most obvious relationships between \( n^{(1)}_{cav} \), \( n^{(2)}_{cav} \), and \( n^{(3)}_{cav} \) are demonstrated in Figure 4-21(b) and Figure 4-21(c). For clarity of presentation, let us consider the initial switching position, Position 0, that can realize the same intermediate orientation of the LC molecules in all cavities, i.e. provide some intermediate value of the refractive index \( n_0 = 1.63 \). We are interested mainly in fine tuning capabilities of the multi-channel filter and, therefore, in small variations of voltage and refractive index \( \Delta n \sim \pm 5 \% \) (red circle, Figure 4-21(a)).

### 4.4.2 Optimal design parameters: Gap Map Approach

Although we have chosen the simplest example of the triple-channel filter, the full investigation of the resonance modes and tuning effects in a wide wavelength range requires a long time for calculations and the data analysis can be complicated in general. The transmission spectra, obtained for different filling fractions \( f_3 \), can reveal certain changes in the positioning, intensity, \( I \), and \( Q \)-characteristics of the resonance peaks. Here, as in the case for single-cavity PhC resonator, it is proposed that the most comprehensive analysis of optical filter properties in general can only be obtained from a combination of TMM and gap map approaches [18, 34, 35]. This combination provides an easy way for graphical engineering of the SBs with multiple resonance peaks in a PhC. This is mainly due to the possibility of selection of different filling fractions, \( f_3 \), and an introduction of any number of cavities during spectra calculations.
following by drawing of all obtained dependences in one graph. Another advantage of the GM approach is that the certain range of $f_{Si}$, for which the optical properties are relatively constant on the graph, provides information about maximum fabrication tolerance of the device.

Figure 4-22: (a) The GM of Si 1D PhC with a triple cavity with $n_{cav}^{(1)}=n_{cav}^{(1)}=n_{cav}^{(2)}=n_{cav}^{(3)}=1.63$ in a wide range of NW. The triple resonances within the first order SB calculated for (b) $f_{Si}=0.1$, (c) $f_{Si}=0.2$, (d) $f_{Si}=0.3$ and $a=573$ nm. The estimated channel spacing, $\lambda_{S12,23}$, and FWHM of each individual resonance are also demonstrated.

In Figure 4-22(a), the GM of the PhC with induced triple defect at the Position 0 ($n_{cav}^{(1,2,3)}=1.63$) is demonstrated. The three transmission channels are realized in a wide range of NW, dividing each SB along the appropriate range of $f_{Si}$. As for the single-
cavity case, the GM demonstrates the narrowing effect of the resonance peaks with increase of the SB’s order, \( m \). Also, the higher order micro-cavities demonstrate higher fabrication tolerances comparing to the lower order cavities, e.g. the 4\(^{th}\) and 5\(^{th}\) order triple-resonance lines are almost vertical as seen from Figure 4-22(a), while the 1\(^{st}\) order triple resonances are more tilted.

In Section 4.3, devoted to investigation of the tuning capabilities of a single-cavity PhC, it was demonstrated, that the higher order SBs are normally more sensitive to the change of the cavity refractive index and demonstrate larger relative tuning shifts of the resonances. All of these properties make the higher order SBs to be the most suitable for the engineering of the tunable multi-resonance devices characterized by the high \( Q \) and narrow FSR.

However, in this Section the investigations are mainly focused on the triple-channel system operating only within the lowest SB of the PhC. This allows establishing the minimum tunability limitations of the suggested methodology. Utilization of the widest resonances, simplifies the presentation of the method, as well as facilitates the monitoring of the filter parameters, e.g. channels spacing, \( \lambda_s \), intensity, \( I \), and bandwidth (full width at half maximum, FWHM, or \( Q \)).

Let us now focus on the first order resonances in Figure 4-22(a) (the region shown by rectangle). The bandwidth of the resonances is very sensitive to the variations of \( f_{Si} \). The most narrow resonance peaks, and, therefore, the strongest coupling between cavities, can be achieved for the range of \( f_{Si} \) that corresponds to the central part of the resonance lines within one SB on the GM (shown by the dashed ellipse in Figure 4-22(a)). In order to perform a detailed analysis, we consider an example of the triple-channel device that operates within the telecommunication wavelength 1555 nm. In accordance with the map, the most narrow first order resonances can be achieved, for example, for \( f_{Si}=0.2 \), which centred at \( NW = 2.5 = \lambda/a \). Thus, the lattice constant of the fabricated device must be design as \( a = 573 \) nm, which corresponds to the width of the air groove/cavity of 458 nm. In Figure 4-22(b) we compare the resonance peaks for the \( f_{Si}=0.2 \) (central part of the resonance lines) and \( f_{Si}=0.1 \) and 0.3 (edges of the resonance lines, outside the dashed ellipse on the GM). Obviously, the resonance peaks for \( f_{Si}=0.2 \) demonstrate the equal channel spacings, \( \lambda_s = \lambda_{s12} = \lambda_{s23} \), the highest out-of-band reflection (\( R=0.99 \)) and the improved bandwidth characteristics (FWHM values are denoted by numbers on each graph).
4.4.3 Fine Tunable filtering of individual resonances

One of the main challenges of the coupled-resonator devices has remained the fixed wavelength channel spacing or free spectral range (FSR), which cannot be easily tuned due to the strong coupling effect between channels. In many applications, the individual channel position (or channel spacing) are required to be trimmed after imperfect fabrication process or to be dynamically tuned for better performance [4]. The tuning of FSR has been demonstrated previously in fiber-based devices [36]. One of the successful attempts was presented in [10], where authors demonstrated their solution for an integrated platform. This approach requires the incorporation of the metallic micro-heaters into the large 245 µm resonators, thus, requiring a precise thermo-control of the device during operation. One of the most promising solutions could be the filter device with low-power and low-loss capability of fine-tuning of individual channels in the whole filtering system in an integrated platform by application of electric field.

4.4.3.1 Precise individual tuning of the central channel in a triple-channel system

It is assumed that the refractive indexes have linear dependence, \( n_{cav}^{(1,2,3)} = n_0 + \Delta n \), demonstrated in Figure 4-21(b). Again, for the clarity of presentation of the method, we assume here, that all cavities are switched to the initial Position 0 (see Figure 4-21), i.e. LC has refractive index \( n_0 = 1.63 \) and the channel spacings between edge channels and the central channel (or FSR) are equal, \( \lambda_{s12} = \lambda_{s23} = 60 \text{nm} \) for the example device with \( a = 573 \text{nm} \) and an optimal value of \( f_0 = 0.2 \). The transmission spectrum of this example structure is demonstrated in Figure 4-23(a) (black line, central resonance denoted by 0).

Now, let us gradually increase the refractive index of the central cavity, \( n_{cav}^{(2)} = n_0 + \Delta n \), by \( \Delta n = 0.001 \), while decreasing the refractive indexes of the two edge cavities, \( n_{cav}^{(1)} = n_{cav}^{(3)} = n_0 - \Delta n \) by the same value of \( \Delta n \) (Figure 4-23(b)). In this case the central cavity has the strongest coupling, \( n_{cav}^{(2)} = n_{cav}^{(1,3)} + 2 \Delta n \), and acts as a primary cavity in the system, while the edge cavities represent the variable mirrors from both sides of the central cavity. At the same time, the overall optical thickness of the system \( n_{cav}^{(1,2,3)} d_{air} \) is decreased, which leads to the blue-shift of its optical characteristics [30, 35]. Let us monitor the positions of triple resonances during these refractive index variations. In Figure 4-23(a) we demonstrate the transmission spectra for the \( \Delta n = 0.013 \) (thin blue line) and \( \Delta n = 0.026 \) (thick blue line). The central channel is blue-shifted,
Figure 4-23: (a) The cavity refractive indexes $n_{cav}^{(1,2,3)}$ versus relative channel position shift normalized to the original channel spacing. (b) Continues tuning of the central channel for $\Delta n=-0.026$ (red dashed line), $\Delta n=-0.013$ (red dashed dotted line), $\Delta n=0$ (black line), $\Delta n=0.013$ (thin blue line) and $\Delta n=0.026$ (thick blue line). (c) The GM of $T=100\%$, calculated for $\Delta n=-0.026$ (red dashed line) and $\Delta n=+0.026$ (blue line). Optimal design region is shown by ellipse.
while the edge resonances have retained their positions. For the considered example, the maximum refractive index difference, $2\Delta n=0.052$ (which is only 24% of the birefringence value for the LC E7, $\Delta n_{E7}=0.2$), allows to achieve maximum relative independent shift of the central channel, $\Delta \lambda_0$, up to 25% of the channel spacing, $\lambda_s$. However, further increase of the overall difference, $2\Delta n$, will break the symmetry of the system and initiates the coupling effect between all cavities resulting in the shift of all resonances simultaneously. As we are interested only in fine tuning capability of the multi-cavity structures, the results obtained for the higher variations of $\Delta n$ are not considered here.

The inverse manipulation with the refractive indexes, i.e. reducing the $n^{(2)}_{cav}=n_0-\Delta n$, while increasing $n^{(1)}_{cav}=n^{(3)}_{cav}=n_0+\Delta n$, results in the individual red-shift of the central channel (Figure 4-23(a), red dashed dotted and dashed lines).

In order to see the independent central resonance tuning in general, the GM is calculated in a wide range of the $f_{si}$ (Figure 4-23(c)). For clarity of presentation we focus only on the first order SB region and plot only regions with $T=100\%$. Here, the resonance lines are calculated only for two limiting cases, namely for $\Delta n=-0.026$ (blue line) and $\Delta n=+0.026$ (red dashed line). Obviously, the widest individual tunability of the central channel can be achieved for the narrowest channels, which corresponds to the optimal central part of the $f_{si}=0.15...0.25$ (denoted by blue circle). This range of $f_{si}$ also demonstrates the maximum fabrication tolerance, which constitutes 54 nm for the example optimal device. The edge resonances remain their original position within the full range of $f_{si}$ for the first SB. Note that the maximum intensity of $T=100\%$ and the initial bandwidths are not affected for all switching positions of the triple-channel system.

4.4.3.2 Precise tuning of the edge channels with high-stability of the central channel

Let us now consider the variation of the refractive index of only the central cavity $n^{(2)}_{cav}=n_0-\Delta n$. The refractive indexes of the edge cavities are considered to be fixed to the initial Position 0, $n^{(1)}_{cav}=n^{(3)}_{cav}=n_0=1.63$ (Figure 4-24(a)). In this case the central cavity plays a role of the variable intermediate mirror between two strongly coupled edge cavities. The decrease by $\Delta n$ of the overall optical thickness of the system
$n_{cav}^{(1,2,3)} d_{air} = \frac{\lambda_{m}^{(1,2,3)}}{2} m$ results in the blue-shift of the edge channels, while the central channel retains its wavelength position. This is clearly demonstrated in Figure 4-24(b) for the $\Delta n=0, 0.02, 0.052$ and $0.11$ for the considered optimized example structure. The increase of the channel spacing, $\Delta \lambda_s$, results in the decrease of the channel spacing between central channel and left edge channel, $\lambda_{s2,3}=\lambda_s-\Delta \lambda_s$, and, consequently, lowering the out-of-band reflection between them.

Similar to the previous model, the overall increase of the refractive index, $\Delta n$, up to 0.052, for the considered example, leads to the linearly proportional change of the channel spacings up to 25%, or $\lambda_{s12} / \lambda_{s23}=1.5$ (Figure 4-24(a, b)). Although the out-of-band reflection between central and right edge channel is decreased, it is still constitutes 95%. Further increase of the $\Delta n$ up to the limiting case, $\Delta n =0.11$, will result in rapidly growing difference between channel spacings, $\lambda_{s12} / \lambda_{s23}$, up to 2.7, with decrease of the out-of-band reflection between the central and left-edge channel down to 90% (Figure 4-24(b), red dashed dotted line).

For significantly higher values of $\Delta n >>0.11$, than considered in this Section, the central cavity acts as a single cavity independent from the edge cavities. The left edge-channel will be shifted out of the SB and the right edge channel will be merged with the central channel, thus changing the resonator mode from triple to a single mode. Obviously, the inverse manipulation with the refractive indexes, i.e. increasing the $n_{cav}^{(2)}=n_0+\Delta n$ and fixed $n_{cav}^{(1)}=n_{cav}^{(3)}=n_0$, results in the individual red-shift of the edge channels on the same $\Delta \lambda_s$ value (Figure 4-24(c)).

In Figure 4-24(d), the GM of the total transmission, $T=100\%$, for the two cases $\Delta n=-0.052$ (blue line) and $\Delta n=+0.052$ (red dashed line) is presented in normalized wavelength range. Again, as for the central tuning combination, the widest tunability can be achieved for the narrowest resonances from the central part of the $f_{st}=0.15...0.25$, which corresponds to the optimal design parameters and minimum fabrication tolerances of the device. Note that the central channel remains its original position within the full range of $f_{st}$ for the first SB.
Figure 4-24: (a) The cavity refractive indexes $n_{cav}^{(1,2,3)}$ versus the ratio of the channel spacings, $\lambda_{s12}/\lambda_{s23}$. (b) Continues blue shift of the edge channels with linear decrease of the central cavity refractive index, $n_{cav}^{(2)}$, by $\Delta n=0.02$ (thin black line), $\Delta n=0.052$ (dashed blue line), $\Delta n=0.11$ (dashed dotted blue line). The triple channels, for $\Delta n=0$, are also demonstrated (thick black line). (c) Continues red shift of the edge transmission channels with linear increase of the central cavity refractive index, $n_{cav}^{(2)}$, by $\Delta n=0.02$ (thin black line), $\Delta n=0.052$ (red dashed line), $\Delta n=0.11$ (red dashed dotted line). (d) The $\text{GM}$ of $T=100\%$, calculated for $\Delta n=-0.052$ (blue line) and $\Delta n=+0.052$ (red dashed line).
4.4.3.3 Precise control of transmission attenuation for the edge channels in triple-channel system

In two previously discussed models, devoted to the realization of fine tuning capability of the triple-defect PhC, the transmission intensities of the realized channels, $I_{1,2,3}$, were substantially stable and close to 100%. In this Section the model for precise engineering of the positions and intensities of the edge channels is demonstrated. This model requires opposite linear variation of the edge channels refractive indexes with the central channel refractive index fixed to the Position 0 (Figure 4-21(c) and Figure 4-25(a)). The mismatch between the optical thicknesses of the edge cavities results in the attenuation of the edge channels intensities, $I_{1,3}$, which accompanied by equal increase of the channel spacing, $x_{si} = x_{23} + x_{31}$ (Figure 4-25(a, b)). By gradual increase of the refractive index difference, $2\Delta n$, the edge channel intensities can be precisely tuned from 100% down to 10%. For significantly higher values of $2\Delta n >> 0.11$, than considered in this Section, the edge channels are vanished and system is operating in single channel mode.

For the case of strongly coupled cavities, when an optimal design value is chosen as $f_{si} = 0.2$, the difference between edge channel intensities $\Delta I_{1,2,3}$ is negligible, and equal to ~1-2 % for all switching modes. However, as it can be seen from the GM in Figure 4-25(c), this difference is significantly increases up to 25 % for all non-optimal values of $f_{si}$ (i.e. values outside the range $f_{si} = 0.15...0.25$; see Section 4.4.2). We note that the attenuation of the resonance intensity for the non-optimal $f_{si}$ is also not so strong in comparison to the optimal device. For example, in Figure 4-25(e), the triple-channel system, calculated for $f_{si} = 0.35$ and $\Delta n = 0.06$, demonstrates a decrease of $I_1$ to 80 % and $I_3$ to 60 %.

One of the possible applications of the controllable transmission attenuation model can be an optimization of the edge channel intensities after fabrication process. The random fluctuation of the geometrical parameters, after the fabrication process, is affecting primarily the edge channels in terms of their intensities and, thus, the bandwidth (or FWHM). The average deviation of the fabricated device parameters up to 10 % may result in the attenuation of the edge channels intensities down to 90 %. By reducing the refractive index mismatch up to $2\Delta n_{car}^{(1,3)} = 0.03$, the edge channel intensities can be precisely tuned back to 100% with negligible decrease of the channel spacing by 1 % (Figure 4-25(e)).
Figure 4-25: (a) The cavity refractive indexes $n_{cav}^{(1,2,3)}$ versus the edge channel intensity $I_{1,3}$ normalized to the maximum original intensity $I_0=I_2$ (lower scale) and versus the relative channel spacing shift normalized to the original channel spacing (upper scale). (b) The precise attenuation of the edge channel intensities, $I_{1,3}$, for $\Delta n=0.015$ (red line), $\Delta n=0.03$ (green line), $\Delta n=0.05$ (blue line), $\Delta n=0.07$ (cyan line) demonstrated for the $f_{si}=0.2$. (c) The GM of $T=25\%$ to $100\%$, calculated for $\Delta n=0.06$. (d) The attenuation of the edge channels for $\Delta n=0.06$ and $f_{si}=0.35$. (e) Fine attenuation from $100\%$ to $90\%$ for $\Delta n=0.005$ (red line), 0.01 (green line), 0.015 (blue line) demonstrated for the $f_{si}=0.2$. 
4.4.4 Design of the SOI-based device

To experimentally demonstrate the proposed idea, the triple-channel resonator device was fabricated on <100> p-type SOI wafer with Silicon device layer thickness of 4.5 μm, and a 1 μm thick buried oxide layer (Figure 4-26). The design parameters of the 1D PhC structures were selected from the GM (Figure 4-22(a)). Electron-Beam Lithography followed by the plasma etching was used to fabricate the nano-scale structures with \( a \) up to 1000 nm based on the first and second order SBs operating in the telecommunication wavelength range. The electrical-isolation of the 2nd, 4th and 6th grooves of 1D PhC is achieved by dry-etching of the micro-channels across the chip (Figure 4-26(a) (green lines) and Figure 4-26(b)). One cone-shape cavity is designed for the easy infiltration of these grooves with LC E7 (Figure 4-26(a) (green region) and Figure 4-26(c)). A 500 nm layer of Aluminum is deposited by sputtering. Then, by using Optical Lithography followed by wet etch process, the contact pads are defined (Figure 4-26(a), yellow circles). Finally, the U-grooves with the depth of 60 μm are

Figure 4-26: (a) The SOI-based chip design of the triple-coupled defect photonic crystal filter filled with nematic LC (green colour) and metal contact pads (yellow circles). (b) SEM image of the fabricated defect-free 1D PhC with three-channels connected to 2nd, 4th and 6th grooves. (c) SEM image showing a view on the channels from the cone-shape cavity designed for LC infiltration.
etched from both sides of the nano-structure for easier integration of the optical lensed fibers and their direct coupling to the device. By independent application of the voltage to the Aluminum contact pads different orientations of the LC molecules can be achieved in the individual grooves, allowing a variety of manipulations of the transmission channels.

4.4.5 Optimization: Compensation of the fabrication tolerances

Any structural deviations and non-uniformities affect the optical properties of the device. In particular, if the periodic structure contains coupled cavities, the thickness deviations, $\delta d$, result in deviation of the optical thicknesses of the cavities, $n\cdot d=n\cdot (d\pm \delta d)$, thus, randomly shifting and attenuating the cavity resonances.

![Figure 4-27](image_url)

**Figure 4-27:** (a) SEM image demonstrates the structural deviations obtained for the defect-free 1D PhC with $a=900$ nm, $f_{Si}=0.4$. (b) Transmission spectra of the originally designed triple-defect device (black line) and of the fabricated device with structural deviations of $\pm \delta d_{Si}=20$ nm (red line). The refractive index of all cavities $n_{cav}^{(1,2,3)}=1.63$. (c) A precise adjustment of the edge channels by decreasing the refractive index to $n_{cav}^{(1,2,3)}=1.60$. (d) Final adjustment of the central channel with $\Delta n=0.01$.

In Figure 4-27(a), one of the fabricated sample PhCs with $a=900$ nm is demonstrated. The original value of filling fraction, $f_{Si}=0.4$, was chosen in accordance with the GM from Figure 4-22(a). After the infiltration of the 2nd, 4th and 6th grooves with nematic LC E7, the PhC tunable filter can be realized. By switching all of the
cavities to the Position 0, the three transmission channels with Q about 500 and centred at $NW=1.75$ (see Figure 4-22(a)), which is $\lambda=NW\cdot a=1715$ nm (Figure 4-27(a), black line), can be achieved. However, the SEM investigation of the fabricated device has demonstrated a presence of the random deviation of the geometrical parameters of the fabricated sample PhC (Figure 4-27(a)). Although, the average width of the grooves, has remained the same for all periods, an estimated average deviation of the thickness of the Si-walls is $\delta d_{Si}=20$ nm, which is about $\pm 5.6\%$ of the originally designed thickness. Therefore, the new optical thicknesses of the cavities can be described as $n_{cav}^{(1,2,3)} (a-d_{Si}\pm \delta d_{Si})$. The obtained transmission spectrum for the fabricated device is demonstrated in Figure 4-27(b), red line. All of the channels are unequally red-shifted which also results in the reduction of Q-factor. The maximum intensity for the edge channels is also reduced by 3-5 %.

Now, let us optimize the fabricated non-ideal system by using the approach demonstrated in this Section. First, we reduce refractive index of all cavities $n_{cav}^{(1,2,3)} = n_0-\Delta n$, in order to blue shift all three channels. The edge channels are precisely adjusted to the ideal positions, when $n_{cav}^{(1,2,3)} = 1.63-0.03=1.60$ (Figure 4-27(c), red line). Now, we perform the fine tuning of the central channel by increasing the refractive index of the edge cavities $n_{cav}^{(1,3)} = 1.61+\Delta n=1.6+0.01=1.61$ and reducing by the same value the refractive index of the central cavity $n_{cav}^{(2)}=1.59$ (Figure 4-27(d)). The system is now fully adjusted to the originally designed operational mode.

4.5 Summary

In this Chapter, the model of transformation of one-dimensional, high-contrast Silicon photonic crystal into a tunable Fabry-Perot resonator has been investigated. This transformation is achieved by introduction of the optical defects in the ordinary photonic crystal while retaining a high modulation of the resonance peaks up to ~0.95.

The features of FP-resonator based on PhC with optical defects are:

i) possibility to avoid the specific procedure for the defects fabrication but rather use the possibility of introducing the filler in the centre of PhC;

ii) tuning of the resonance peaks within the PBG by variation of refractive index of the defect filler.
The utilisation of common GMs of PBGs (or stop-bands) and TBs allows to predict the resonance appearance or disappearance in the optical spectra and to determine the optimal design parameters, e.g. wavelength position, quality factor and free spectral range depending on the order of PBG and the value of filling fraction.

- **Single-cavity resonator: Wide-tuning of the resonances**

  A Fabry-Pérot resonator, consisting of two Silicon walls, also acting as electrodes, and a thick cavity, filled with the nematic liquid crystal E7, was fabricated on a Si-On-Insulator platform. The experimental spectra obtained are in good agreement with the results of calculations based on GM Method. In particular, a superposition of the transmission peaks with reflection maxima, predicted from calculations, was confirmed experimentally. Altering the liquid crystal alignment, and consequently the refractive index value in the cavity, by the application of an electric field using voltages from 0 V to 15 V, results in reversible continuous tuning of the high-order resonance peaks with the ultra-wide relative shifts of up to $\Delta \lambda/\lambda \approx 10\%$.

- **Triple-cavity resonator: Individual tuning of resonances**

  A technique for precise position control of individual transmission channels/resonances in a triple-cavity resonator device has been proposed. By controllable tuning of the refractive index in all coupled cavities, a continuous individual tuning of the central channel (or edge channels) up to 25% of the total channel spacing has been demonstrated. Additionally, an approach for precise controllable improvement of transmission up to 100% is demonstrated for the edge channels with decrease of the channel spacing on-1%. Based on the proposed design, a prototype triple-channel filter was fabricated on Silicon-On-Insulator platform and optimized to the desired operational mode. The suggested approach has been utilized for compensation of the fabrication tolerances in multi-channel Silicon devices in a wide infrared range.

  This project is currently going through the final fabrication process at Tyndall Institute Ireland (NAP368 funded by SFI Ireland).
4.6 References

[22] M. KGaA, [Data Sheet Licristal® E7], Germany(2001).


Chapter 5.

Photonic Crystals with Structural Fluctuations

5.1 Introduction

Although Si fabrication technology has significantly developed over the last 20 years, one of the main problems for optical, micro- and nano-scale, periodic structures, such as photonic crystals, remains defining the maximum structural deviations precisely in the system [1-3]. In general, structural deviations and non-uniformities, presented in the patterned features on the wafer, occur for three principal reasons. First of all, there is the fundamental diffraction limit of the projection optics. Secondly, the mask pattern differs from the original design due to limitations in the mask fabrication process. Finally, random and systematic variations inevitably occur in a multitude of lithographic process parameters, such as focus and exposure [4]. Fabrication tolerances for modern e-beam lithography are usually assumed to be a minimum of about 5-10% of the nominal target dimensions. The question arises as to how imperfections in the fabricated 1D PhC structure might influence their optical properties? Answering this question requires the development of a mathematical model of the multilayer structure. Once this model is validated, the response of the optical properties of the system to fluctuations in the structural parameters is estimated. When modelling a 1D PhC, four main structural parameters are involved. These are, the thicknesses, $d_{hi}$ and $d_i$, and the
refractive indices, $n_H$ and $n_L$, of the high and low refractive index components, respectively (Figure 5-1). The sum of $d_H$ and $d_L$ is $a$, the lattice constant of the PhC.

Another structural imperfection that can occur at certain level in practical 1D PhC structure fabricated by a microstructuring process [5], is a roughness of the side-walls of etched air channels. Depending on the aspect ratio and particular method used, the surface roughness can be varied from 0.4% to 20% of the Si wall thickness during reactive ion etching, from 10% to 15% during photo-electrochemical etching and <1% during anisotropic chemical etching (see Chapter 2). Technological deficiencies resulting in side-wall roughness in 1D PhCs were investigated in Refs. [6-10], whereas in Refs. [6, 8, 11-12], non-uniformities in wall thickness were analysed. The investigation of the influence of fluctuations in the geometrical parameters, or PhC disorder, on the optical properties of PhCs is a crucial aspect of material engineering, since this allows an estimation of the maximum level of disorder, beyond which the optical properties of the crystal are unacceptably degraded. For example, in Ref. [13], the threshold level of disorder below which the probability of formation of an eigenstate at the center of a PBG is negligible was established. Introduction of disorder into a 2D PhC as a result of the variation in the size of the air cylinders leads to increasing transmission within the PBG and to a distortion of the PBG’s shape [13]. The PBG width is used as a metric to describe this distortion. The width can be determined as the distance between the boundaries of areas on dispersion curve where the Bloch wave vector $K$ has imaginary values [14].

Figure 5-1: Schematic diagram of a seven-period, 1D PhC with a lattice constant $a=d_H+d_L$ and an optical contrast of $n_H/n_L$. A wall thickness with fluctuation ($d_{fl}$), in the
H-component appears in each lattice period, causing a variation \((d_{ij})\) in the L-component of the structure.

Typically, 1D PhCs are designed as Bragg reflectors with the optical thickness of both layers, \(d_{n_H}n_H\) and \(d_{n_L}\), corresponding to the quarter wavelength for which this PhC is going to be utilized. In addition to the first PBG, one-dimensional PhCs have numerous secondary and higher orders, PBGs. These have been investigated in Refs. [10, 15], for example. Utilisation of secondary and higher order PBGs allows number of applications of 1D PhCs, including Fabry-Pérot optical filters with tunable resonance peaks of high-order (Chapter 4), or the formation of wide-band windows of transparency in Si (Chapter 3). For these structures [16, 17], a large variation of filling fractions, \(f_{n_H} = d_{n_H}/a\) or \(f_{n_L} = d_{n_L}/a\), was used, unlike conventional structures based on quarter wavelength optical thicknesses.

In this Chapter, the influence of disorder on 1D PhCs of high optical contrast for use in Si photonics is investigated. Using a combination of calculations and gap map analysis, the influence of random thickness fluctuations in PhC parameters on the transmission spectra and PBGs is explored. The advantage of using PBGs map approach is that it enables the analysis of the optical properties of the PhCs over a range of possible filling fractions and photonic band gaps of any order, including the most common quarter wavelength structures.

### 5.2 Calculations of spectra and PBG map

A two-component 1D PhC with thicknesses of \(d_{n_H}\) and \(d_{n_L}\) for the high \((n_H)\) and low \((n_L)\) refractive index components, respectively, and a total of seven periods is shown in Figure 5-1. During microstructuring processes such as lithography and wet or dry etching, the optical constants of the constituent materials generally remain unchanged. We use an \(n_H\) value for Si in the mid-IR range of 3.42 and a value of \(n_L = 1\) for the air component of the grooved Si structure. Figure 5-2(a) shows the reflection spectrum \(R\) at normal incidence of light, calculated for a filling fraction \(f_{n_H} = d_{n_H}/a = 0.23\), corresponding to a quarter wavelength optical thickness for both components. Wavelength values, \(\lambda\), are shown in units of normalized frequency, \(a/\lambda\), on the x-axis. Reflection spectra calculated for \(f_{n_H} = 0.5\) and \(f_{n_H} = 0.08\), are shown in Figure 5-2(b) and Figure 5-2(c), respectively. Wide reflection bands with a characteristic Π-shape, corresponding to the first and higher order PBGs, are seen in all of the \(R\) spectra.
Figure 5-2: (a), (b), (c) $R$ and (d), (e), (f) $T$ spectra of an ordered PhC based on a "Si-air" structure for (a), (d) $f_H=0.23$; (b, e) $f_H=0.5$ and (c, f) $f_H=0.08$. The number of lattice periods, $N=7$, the incoming and outgoing medium is air and a normal incidence of light is used for these calculations. The numbers correspond to the order number of the PBGs from Figure 5-3.

From Figure 5-2(d,e,f) it is clear that within the PBG’s frequencies, the very pronounced dips in transmission indicate that amplitude modulation of up to $\sim 80$ dB in the $T$ spectra are possible. (Note the log scale on the $y$-axis). For comparison, the amplitude modulation of $T$ outside the PBG regions is around 10 dB. These dips can be
explained by the appearance of the imaginary part of the wave vector, $K$, in the range of PBGs frequencies [14]. The imaginary part of the wave vector $K$ affects the spectrum in a way which is equivalent to strong absorption of the light. The light is not absorbed via the usual electronic route within the atoms of the material. Rather, it is due to a strong interaction of the incident light with the periodic structure. Clearly, the boundaries of the strong dips are the boundaries of PBGs. The transmission spectra and PBG map will be further used for the evaluation of the impact of thickness fluctuations on the optical properties of PhCs.

![Figure 5-3: Gap Map for ordered PhC, based on "Si-air" structure, with N=7. The lines, intersecting the PBG regions labelled with the numbers shown, are demonstrated for $f_h = 0.23$ (dashed line), $f_h = 0.08$ (dotted line) and 0.5 (short dotted line).](image)

The main (or 1st) PBG and a number of PBGs of high order, labelled 1 to 14, are observed on the gap map in a wide range of filling fractions in Figure 5-3. It can be seen that for the number of periods here ($N=7$), the 1st PBG with $R>0.99$ can be obtained in the range $f_h = 0.04-0.7$. The PBGs of higher order number occupy smaller areas on the map. The filling factor $f_{Si} = 0.23$ corresponds to $\lambda/4$ optical thicknesses for
each PhC component. Note that the maximum width of the 1st PBG is at this value of $f_{Si}$, marked with a dashed line on the map. We are also interested in the high-order PBGs, for example, the regions numbered 2-9. The widest part of the second PBG corresponds to $f_{Si} = 0.5$, the associated $R$ spectrum is presented in Figure 5-2(b). The widest part of the third PBG corresponds to $f_{Si} = 0.08$, the associated $R$ spectrum is presented in Figure 5-2(c).

The width of the 3rd PBG is larger than the width of the 1st PBG. Therefore, this PBG can be used as a wide-band reflector, with the width of the $R$ band being larger by a factor of 1.3 than the $R$-band of the reflector with an optical thickness of the components equal to $\lambda/4$.

### 5.3 Modelling of thickness fluctuation

During the fabrication of PhCs, the tolerance in the lattice period of the ordered structure $a = d_H + d_L$ is determined by the lithographic accuracy, which is typically high. However, if an inaccuracy, for example, in the thickness of one of the components, $d_H$, occurs as a result of process variations, this will lead to an inaccuracy in the thickness of the second PhC component, $d_L$ (Figure 5-1). Note that technologically all layers in these periodic structures are fabricated simultaneously and, therefore, it is impossible to make any alterations to the final structure. This is not the case for thin film coatings, where the periodic structure is formed by sequential deposition.

Let the number of walls in a PhC be $i=8$ as shown in Figure 5-1. In order to draw the PBG map, it is necessary to first calculate the spectra $R$ (or $T$) in a range of values of $d_H$ from 0 to $a$. Next, let us introduce the standard deviation, $\delta$, as a parameter which is related to the wall thickness, $d_H$, in the ordered PhC and leads to the inaccuracy, or relative fluctuation, $\delta_i$, induced in the $i^{th}$ wall of the ordered structure in accordance with the random distribution law.

We will use two approaches to account for the thickness fluctuation $\delta d_H$. The first approach consists of the introduction of fluctuations proportional to the thickness of the $i^{th}$ wall. Thus, the value of the fluctuation increases with an increase in the wall thickness. In this case, the thickness of the $i^{th}$ wall, $(d_H)_i$, in the presence of a thickness fluctuation $\delta d_H = \delta_i d_H$, is determined from the following Equation (5.1):

$$
(d_H)_i = d_H + d_H \cdot \delta_i = d_H (1 + \delta_i)
$$

(5.1)
In the second approach, the thickness fluctuation is determined by equation \( \delta d_{it} = (d_{it})_{\text{min}} \cdot \delta_i \), where \((d_{it})_{\text{min}}\) is some minimal value of the wall thickness. In this case the value \((d_{it})_{\text{min}}\) changes in accordance with equation (5.2):

\[
(d_{it})_i = d_{it} + (d_{it})_{\text{min}} \cdot \delta_i \quad (5.2)
\]

Let us select the value of \((d_{it})_{\text{min}},\) corresponding to the filling fraction \(f_H = 0.08\). Eqn. (5.2) transforms to Eqn. (5.3):

\[
(d_{it})_i = d_{it} + 0.08 \cdot a \cdot \delta_i \quad (5.3)
\]

For example, using the first approach and standard deviation, \(\delta=0.05\), if the value of the relative fluctuation \(\delta=0.11\) (for \(i =1\) in Table 5-0-1) then the thickness fluctuation will correspond to 0.11\(d_{it}\). For \(a=3\ \mu m\) at a lower value of \(f_H = 0.1\), the thickness \(d_{it}\) will be equal to 0.3 \(\mu m\), while at a higher value of \(f_H=0.7\), the value of \(d_{it} = 2.1\ \mu m\). The calculated thickness fluctuations \(\delta d_{it}\), determined from Eqn. (5.1), are 0.3\(0.11 = 0.033\ \mu m =33\ \text{nm}\) and 2.1\(0.11 =0.231\ \mu m =231\ \text{nm}\), respectively, i.e. \(\delta d_{it}\) will be proportional to the thickness of the walls. Using the second approach, if \(\delta = 0.1\), for the selected lower value of \((f_H)_{\text{min}} = 0.08\), the value of the thickness fluctuation \(\delta d_{it}=24\ \text{nm}\) at \(a=3\ \mu m\), and therefore, all other walls thicknesses in the range of the filling fraction from 0 to 1 will have fluctuations of 24 nm. Therefore, the difference between the approaches 1 and 2 is that in the first case we are dealing with more radical changes in thickness fluctuation \((d_{it})_i\), while in case 2 the thickness fluctuation is less pronounced.

For both approaches, we use a random-number generator, which, based on a standard deviation of \(\delta\), generates for each \(i^{\text{th}}\) wall, a value of \(\delta_i\) in accordance with the normal random distribution law. Using Equations (5.1-3), we obtain the variation of thickness in each \(i^{\text{th}}\) wall as \((d_{it})_i\). Since actual values of \(\delta_i\) can be either positive or negative, the thicknesses \((d_{it})_i\) can be either smaller or larger than \(d_{it}\) in an ordered PhC. As an example, histograms for 12 types of thickness fluctuation distribution for a structure with eight walls (Figure 5-1) with \(\delta=0.05\) are presented in Figure 5-4.
Figure 5-4: Histograms for 12 types of thickness fluctuation distribution values $\delta_i$ for an eight wall PhC with standard fluctuation $\delta=0.05$.

5.4 PhC with thickness dependent variations in the wall thickness

Let us consider in detail the first approach using, as a model, a PhC with eight walls (i.e. $i=8$) as shown in Figure 5-1. For the first type of distribution (type 1) the dependence of the values of $\delta_i$ on the wall number is presented in Figure 5-4. The thickness fluctuation $\delta_i$ and the thickness $d_{11}=0.66 \mu m$ (corresponding to $f_{11}=0.23$ for a PhC with $d=3 \mu m$) are presented in Table 5-0-1 along with the altered values of wall thickness $(d_{11})_n$, taking into account the relative fluctuation $\delta_i$.

Now that the new values of $(d_{11})_n$ are known, a calculation of layer thickness $d_i$, the distance between the walls in Figure 5-1, can be performed. Since in our model, $a$ has a constant value, i.e. the distance between the centres of the walls remains unchanged, the new value of the distance between the two walls (for example walls 3 and 4) will correspond to the difference $(d_i)_{34}$, determined by Equation (5.4):

$$(d_i)_{34} = a - [(d_{11})_3/2 + (d_{11})_4/2] \tag{5.4}$$
Figure 5-5: Gap maps of an a) ordered (thin line) PhC (from Figure 5-3) and a disordered (thick line) PhC with standard random thickness deviation of the walls of $\delta=0.05$. The fluctuation distribution used is type 1 from Figure 5-4(a). (b) Gap maps under identical conditions to those in figure (a) but with fluctuation distribution of type 8 (Figure 5-4(h)) and (c) type 6 (Figure 5-4(f)). Wall fluctuations are proportional to wall thickness. The dashed line corresponds to $f_H=0.23$ and the dotted lines correspond to $f_H = 0.08, 0.5$ and 0.71.
Table 5-0-1: Dependence of the relative fluctuations $\delta_i$ (for distribution of type 1) on the wall number and wall thickness values $(d_{H,i})$ for a standard deviation of $\delta=0.05$. Values are given for an eight-wall structure in a PhC with $d_H=0.66 \mu m$ $(f_H=0.23, a=3 \mu m)$.

<table>
<thead>
<tr>
<th>i</th>
<th>Values of fluctuation $\delta_i$</th>
<th>Values of thickness for $i^{th}$ wall $(d_{H,i})$, $\mu m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.110</td>
<td>0.732</td>
</tr>
<tr>
<td>2</td>
<td>0.040</td>
<td>0.687</td>
</tr>
<tr>
<td>3</td>
<td>0.049</td>
<td>0.693</td>
</tr>
<tr>
<td>4</td>
<td>0.043</td>
<td>0.688</td>
</tr>
<tr>
<td>5</td>
<td>0.046</td>
<td>0.690</td>
</tr>
<tr>
<td>6</td>
<td>0.023</td>
<td>0.682</td>
</tr>
<tr>
<td>7</td>
<td>-0.052</td>
<td>0.626</td>
</tr>
<tr>
<td>8</td>
<td>0.003</td>
<td>0.662</td>
</tr>
</tbody>
</table>

Next, taking into account the changes in all of the thicknesses, $d_H$ and $d_L$, we perform a calculation of the gap map taking into account the thickness fluctuations. Using the approach suggested earlier for an ordered PhC (Figure 5-3), we use the criterion $R>0.99$ and draw the gap map for the disordered PhC with a thickness fluctuation of type 1 and a value for $\delta=0.05$. In Figure 5-5(a) we present both maps on the same graph. From Figure 5-5(a), the position of the PBGs regions for ordered and disordered PhCs with $\delta=0.05$ for lower values of $f_H$ are practically the same, while at higher $f_H$ values the PBGs are shifted to smaller $a/\lambda$ values, that is, a red shift.

Let us analyse in detail what happens with the $T$ spectra for a few values of $f_H$ (Figure 5-6). From Figure 5-6(a), for $f_H=0.08$ there are no changes visible in the dips in the $T$-spectra within the same frequency range. For $f_H=0.23$, a red shift of the PBGs begins to become apparent, which increases when $f_H$ is increased to $f_H=0.5$ and 0.71 (Figure 5-6 (b, c, d)). In parallel with this shift, a distortion in the shape of the high-order PBGs also occurs.
Figure 5-6: Transmission spectra $T$ for ordered (black line) and disordered (grey line) PhCs with filling fractions a) $f_{H} = 0.08$, b) 0.23, c) 0.5, d) 0.71, with corresponding thickness fluctuations $\delta d_H = 0.004a$, 0.0115$a$, 0.025$a$ and 0.036$a$ and fluctuation distributions of type 1 from Figure 5-4(a) and Table 5-1. Numbers inside the dips (PBGs) correspond to the number of the PBG shown on the gap map in Figure 5-5(a).

A shift in the PBG regions, and a change in the $T$ spectra, typically occurs for a small change in filling fraction, $f_H$. Analysing the distribution of thickness fluctuations in Figure 5-4 and Table 5-0-1, it is apparent that nearly all $H$-layers increase their thickness ($d_H$), when compared with the ideal case of $d_H = 0.66 \mu$m. Evidently, the filling factor has changed. The increase of ($d_H$) here generates a red shift in the PBG on the map and in the $T$ spectra. A proportionate dependence of the increase in PBG edges with an increase of $f_H$ is observed, which can be explained by the increase in the optical thickness of the altered $H$-layers and their bands in the $T$ spectra (Figure 5-6(c)) and its increasing influence with an increase in filling fraction $f_H$. 
Figure 5-7: T spectra for ordered (black line) and disordered (grey line) PhC with fluctuation distribution of type 8 for a) $f_H=0.23$ and b) $f_H=0.5$ with thickness fluctuations $\delta d_H = 0.0115a$ and $0.025a$, respectively.

From the fluctuation distributions, shown in Figure 5-4, the fluctuation type 8 was selected and used to calculate the $T$ spectra for two values of $f_H$, a low $f_H=0.23$ and a high $f_H=0.71$ (see Figure 5-7). It is apparent that the distortion of the PBG occurs without a frequency shift outside the PBG band in ordered PhCs. If the fluctuation type 8 is used, it does not lead to a shift in the PBG as a function of filling fraction. This conclusion is supported by calculations using fluctuation type 8, presented in Figure 5-5(b), which demonstrates that distortion of PBGs occurs with increasing order without an associated shift in the PBG regions.

Figure 5-4 also shows fluctuation type 6, which demonstrates an approximately even distribution of $\delta$ on $i$ around the middle line (at $y=0$), but with a pronounced single fluctuation within one of the internal walls, namely the 6th wall. The gap map calculated for this distribution type, is shown in Figure 5-5(c). Analysing this gap map, it is apparent that disorder does not result in a shift of PBGs, however characteristic narrow-band regions within the PBG regions have appeared, either in the centre or at the edges.
Let us select a PBG where the influence of thickness fluctuations is easily observed, for example, in the case of $f_{H}=0.23$ and $f_{H}=0.5$. For these values of $f_{H}$, the well-modulated transmission dips in the $T$ spectra correspond to the $1^{\text{st}}$ and the $5^{\text{th}}$ PBGs in Figure 5-8(a) and the $1^{\text{st}}$, $2^{\text{nd}}$ and $4^{\text{th}}$ PBGs in Figure 5-8(b). The narrow peaks within the dips in the $T$-spectra are related to the defect modes. When these peaks are close to the PBG edges, they deform the edges of PBGs and a decrease in the modulation of the amplitude of $T$ within the PBG region occurs simultaneously. The distortion of the PBG in the $T$ spectrum caused by thickness fluctuations is more pronounced for the higher band orders.

From Figure 5-6, 7, 8 it can be seen how the interference fringes between PBGs change. They increase in the $T$ spectra with an increase in the PBG order. This is also a result of the introduction of thickness non-uniformities into the PhC. If a simultaneous degradation of the edges also occurs, then determining the position of the PBG boundaries becomes problematic. As the band number increases, these effects intensify, increasing the difficulties in determining the PBG’s width.
Figure 5-9: Gap map of ordered (black line) and disordered (grey line) PhC with a standard deviation in thickness $\delta=0.2$ and fluctuation distribution of type a) 1 and b) 6. The value of the fluctuation $\delta d_H=0.016a$ is constant for different wall thicknesses.

5.5 *PhC with a constant value of fluctuation for all wall thicknesses*

Let us consider a second approach for the introduction of thickness fluctuation values, using a minimal thickness deviation for all filling fractions $f_{Ht}$. Absolute fluctuation values from Eqn. (5-2) will correspond to $\delta(d_H)_t=12, 24$ and 48 nm for $a=3$ µm and $f_{Hmin}=0.08$ for the corresponding three values of $\delta=0.05, 0.1$ and 0.2 for two types of fluctuation distribution, viz. type 1 and type 6. Differences in the position of the PBG regions on the maps for ordered and disordered PhC with fluctuations of type 1 are negligible up to $\delta=0.05$ ($\delta d_H=0.004a$). For $\delta=0.2$ ($\delta d_H=0.016a$) these become apparent (Figure 5-9(a)) as a shift of the PBG region edge, this shift is more pronounced for PBGs of high order. We can explore this further by analyzing the dips in the $T$ spectra for various values of $f_{Ht}$ (Figure 5-10). In this model, the same red shift will be observed in all spectra with different values of $f_{Ht}$. This red shift was discussed earlier in relation to Figure 5-5(a) and Figure 5-6. These shifts are explained by the nature of the fluctuation distribution, which increases the filling fraction at the expense of wall thickness.
Figure 5-10: $T$ spectra of ordered (black line) and disordered (grey line) PhC with fluctuations of type 1 for a) $f_{H}=0.08$, b) $f_{H}=0.23$, c) $f_{H}=0.5$ and d) $f_{H}=0.71$. The value of the thickness fluctuation $\delta d_{H}=0.016a$ is constant for different wall thicknesses.

For the fluctuation type 6, it can be seen from Figure 5-9(b) that changes in the PBG regions are observed as a result of the introduced fluctuation with $\delta=0.2$. The boundaries of the regions are not shifted, but defect peaks have appeared within the PBG's frequencies. The same effect is observed in the $T$ spectra (Figure 5-11). For example, in Figure 5-11(b) for $f_{H}=0.23$, the shape of the 1st PBG is partially distorted due to the appearance of a defect peak near its edge. The presence of the defect peaks, as discussed earlier, can be explained by the type of fluctuation 6, in which the dominant thickness deviation is present near the centre of the PhC.

During our investigations of the influence of other types of thickness fluctuation shown in Figure 5-4 (i.e. types 2-5, 7-8 and 10-12) we observed that the boundaries of the PBG regions in the disordered structures are not shifted. Their behaviour is generally similar to that of type 8 (see the analysis of Figure 5-5(b) and Figure 5-7), because this type of thickness fluctuation demonstrates broadly similar positive and negative thickness fluctuations.
Figure 5-11: T spectra of ordered (black line) and disordered (grey line) PhC with fluctuation distribution of type 6 for a) $f_H=0.08$, b) $f_H=0.23$, c) $f_H=0.5$ and d) $f_H=0.71$. The value of the thickness fluctuation $\delta d_H=0.016a$ is constant for different wall thicknesses.

Analysing the shift of PBGs regions from Figure 5-9(a, b), it is clear that the shift does not depend on filling fraction, i.e. on thickness of $d_H$. Therefore, only the amount of thickness fluctuation introduced into the PhC influences the bands shift. This conclusion is confirmed by the increase in the PBG shift noted above, together with an associated shift in the spectra, as a consequence of increasing thickness fluctuation from $\delta d_H=0.004a$ to $0.036a$ (Figure 5-6).

5.6 Summary

A combination of mathematical modelling and gap map analysis allows the influence of randomly induced thickness fluctuations in photonic crystal components on the distortion of photonic band gaps in one-dimensional PhCs to be investigated. The investigation of band gaps in the transmission spectra provides further, detailed information on the influence of thickness fluctuations. In this study, 1D PhCs based on microstructured semiconductors “Si-air”, with a range of filling fractions and PBGs of
different order was studied. Three characteristic types of fluctuation distribution and
two ratios of the fluctuation parameters to the wall thicknesses were considered. By
introducing thickness disorder into the PhC, and depending on the type of fluctuation
distribution, a shift of the PBGs, the appearance of defect modes, a decrease in the
amplitude modulation of transmission within the PBG and an increase in interference
fringe modulation between PBGs were observed.

We established that the change in the PBGs depends on the magnitude of the
fluctuations and increases with an increase in the order of the PBG. Introducing
thickness non-uniformity into the PhC of up to 0.004 from value of lattice constant $a$ for
different types of fluctuation distribution has almost negligible effect on either the
position or the shape of the 1st and nearest PBGs. However, depending on the type of
fabrication, whether the optical or e-beam lithography is used, the effect can be larger or
smaller. For example, the e-beam lithography provides small fabrication error (Chapter
4; Section 4.4.5), while the classical optical lithography, used for the fabrication of
structures with $a>1$ μm, gives significantly higher fabrication errors. The approach
presented here enables the determination of the fabrication tolerances required for the
geometrical parameters of the PhC structure and allows optimisation of the design of
these structures for the utilisation of high order PBGs, including structures with PhC
components with quarter wavelength optical thicknesses. This approach is also useful
for the solution of the complementary task, the determination of the parameters of the
PhC structure from it’s reflection/transmission spectra.
5.7 References


Chapter 6.

Conclusion

This thesis has been concerned with the design, fabrication and optical investigation of novel photonic crystal structures for application in integrated Silicon microphotonics. The studies undertaken yield information on the new unique optical properties of the developed multi-component as well as single- and multi-cavity photonic crystals based on grooved Silicon for in-plane light modulation.

The basic concepts underlying the photonic crystal optical properties and their modifications have been demonstrated in Introduction Chapter. A classical transfer matrix method and gap map approach have been elaborated and applied to mathematically describe and design the one-dimensional photonic crystals structures based on Silicon. The viability of the results achieved in this thesis is confirmed by experimental results as well as by comparison with previous results reported by other authors. For experimental technological realization of the proposed free-space photonic crystal structures the classic optical and e-beam lithography as well as wet and dry etchings of (100) and (110) Silicon were utilized. The optical characterization was performed in a wide infrared spectral range using the Fourier Transform Infrared microspectroscopy (1-15 μm) and optical fiber-coupling set-up based on optical spectrum analyzer (1.2-1.7 μm).

The effects demonstrated have practical applications in integrated Silicon microphotonics. The suggested photonic crystal models can be applied to the design of any micro- and nanostructured semiconductor or dielectric material for application across the entire electromagnetic range.
Multi-component Photonic Crystal structures

Utilisation of a multi-component photonic crystal by the introduction of an additional regular material into a grooved Silicon structure, while leaving the lattice constant unchanged, provides a suitable model for designing a new type of photonic crystal. Use of a gap map allows visualization of the transformation of the photonics band gap areas caused by converting an ordinary two-component PhC to a three-component PhC by the addition of the new regular layer. The introduction of the third component to the 1D PhC enables variation of the PBGs areas of the three-component PhC and, therefore, engineering of the optical contrast of the original two-component PhC. This is achieved, not by filling its air channels, but by selecting either the thickness or the refractive index of the third layer. Using the approach suggested for decreasing the optical contrast in photonic crystal, the omni-directional bands can be obtained in a high-contrast “Si-air” periodic structure. A number of simulated models of three-component 1D photonic crystals are described, some of which may have practical applications.

For the first time the principle of suppression of the PBGs and replacing them with transmission bands (TBs) is demonstrated for a high contrast 1D PhC with the introduction of an additional layer. By varying the thickness of this layer, the width and the number of the TBs can be altered. The TBs obtained numerically show a high transmission value (>99 %) and a substantial band width in the infrared spectral range. The GM approach was used to generate the map of transmission bands in order to observe the effect in the entire range of Si filling fraction and in a wide wavelength range. The generated maps of TBs have demonstrated the formation of the ultra-wide transmission bands over the suppressed PBGs in a whole range of possible filling factors. The TBs obtained demonstrate a substantial bandwidth (>200 nm) and a negligible number of ripples within the bands. For the certain angles of incidence of light the multi-component PhC devices demonstrate the polarization effect: the remaining PBGs for one-polarization may overlap with the obtained wide TBs for another polarization, therefore transforming the PhC into a broadband polarizer. In order to fine tune the wavelength position, number and width of the output transmitting or reflecting bands, thermal oxidation of the grooved Si structures was exploited. Based on the generated map of TBs the PhC filter with ultra-wide TB characteristics has been successfully fabricated and characterized. The TB obtained exhibit a high transmission
of 92-96% and a substantial bandwidth of 1800 nm with negligible number of ripples on the top.

**Microcavity Photonic Crystal Structures:**

The model of transformation of one-dimensional, high-contrast Silicon photonic crystal into an efficient tunable Fabry-Perot resonator in which a wide Stop Band is used for frequency resonance separation has been proposed and investigated. This transformation is achieved by introduction of the optical defects in the ordinary photonic crystal by infiltration of certain periods with refractive index matching filler.

The FP-resonator based on PhC with optical defects has a number of significant advantages from the practical point of view. These are, for example, the possibility to avoid the specific procedure for the defects fabrication but rather use the possibility of introducing the filler in the centre of PhC and tuning capability of the resonance peaks within the SBs by variation of the refractive index of the defect filler.

The utilisation of common gap maps of PBGs (or stop-bands) and TBs allows to predict the resonance appearance or disappearance in the optical spectra and to determine the optimal design parameters, namely the wavelength position, the quality factor and the free spectral range depending on the order of PBG and the value of filling fraction.

By using nematic liquid crystal E7 as a filler, the precise continuous tuning of the obtained resonances was experimentally achieved by either varying the temperature from 10° to 65°C or by application of electric field from 0 to 15 V. The obtained result has demonstrated the largest experimental shift, achieved up to date for the microstructured resonators based on Si and Liquid Crystal (LC), and utilized for molding of light propagated parallel to the substrate. It was also shown theoretically and experimentally, that for the high optical contrast structure on Silicon the reflection from Si wall is reached the value of ~0.95, that provide a high quality resonance peaks in a wide range of spectra, measured from 1.5 to 15 μm. Most importantly it was established that a significant shift of peak position is achieved by using the resonance peaks of high order. In particular, a superposition of the transmission peaks with reflection maxima, predicted from calculations, was confirmed experimentally.

For the first time, an electro-optical technique for precise position control of individual transmission channels/resonances in a triple-cavity resonator device has been
proposed. By controllable tuning of the refractive index in all coupled cavities, a continuous individual tuning of the central channel (or edge channels) up to 25% of the total channel spacing has been demonstrated. Additionally, an approach for precise controllable improvement of transmission up to 100 % is demonstrated for the edge channels with decrease of the channel spacing on ~1 %. Based on the proposed design, a prototype triple-channel filter was fabricated on Silicon-On-Insulator platform and optimized to the desired operational mode. The suggested approach has been utilized for compensation of the fabrication tolerances in multi-channel Silicon devices in a wide infrared range.

Influence of the thickness fluctuations on PBG properties:

The influence of randomly induced thickness fluctuations in photonic crystal components on the distortion of photonic band gaps in one-dimensional PhCs has been investigated in detail. Three characteristic types of fluctuation distribution and two ratios of the fluctuation parameters to the wall thicknesses have been considered in this study. By introducing thickness disorder into the PhC, and depending on the type of fluctuation distribution, a shift of the PBGs, the appearance of defect modes, a decrease in the amplitude modulation of transmission within the PBG and an increase in interference fringe modulation between PBGs have been obtained. The change in the PBGs depends on the magnitude of the fluctuations and increases with an increase in the order of the PBG. Introducing thickness non-uniformity into the PhC of up to 0.004 from value of lattice constant for different types of fluctuation distribution has a negligible effect on either the position or the shape of the first and nearest PBGs. The developed mathematical approach presented here allows the determination of the tolerances required in the geometrical parameters of the PhC structures during fabrication. It also allows the optimization of PhC structures using high order PBGs.

The scientific novelty of the work:

• The full and systematic analyses of the optical characteristics of the in-plane one-dimensional multi-component photonic crystal structures and micro-cavity photonic crystals filters have been developed and proposed using the gap map approach.
• The model of a three-component PhC was developed and the approach for engineering of the optical contrast by variation of the additional component thickness was suggested and experimentally demonstrated.

• For the first time, the regions of transparency in multi-component PhC have been discovered and experimentally demonstrated for the three-component PhC based on "Si-SiO₂-air" structure with bandwidth of the flat-top pas-bands of 1800 nm.

• The utilization of common maps of stop-bands and pass-bands allows extensive analyse of the discovered effect of total transparency in Silicon based photonic crystals. The full suppression of the certain order stop-bands and their replacement with wide-band pass-bands have been demonstrated.

• The reverse continuous electro-tuning of the LC director orientation from spontaneous planar to homeotropic has been achieved and demonstrated for the defect-free PhC FP-resonators based on SOI platform. An outstanding experimental wide shift of 10 % of the resonance peaks has been successfully demonstrated. This is the largest resonance shift achieved to date in Si photonic crystals.

• For the first time, the compact and integratable solution for multi-channel photonic crystal filter with fine-tuning capability of individual channels up to 25 % is demonstrated.

**Summary of the potential applications of the methods used in this work:**

• For the first time, the Gap Map approach proposed as a core engineering tool for photonic crystal based devices, such as resonators and ultra-wide band-pass filters. From the theoretical point of view, the determination of the optimal design parameters using the GM approach in the entire range of wavelength and filling fraction provides deeper understanding of the physical processes in photonic optical devices. From the fabrication point of view the developed gap maps here allow highly accurate determination of the fabrication tolerances of the photonic crystal structures.

• The transfer matrix method source code developed for multi-component and micro-cavity PhC structures in MathCad and Matlab Software during the doctoral work can be used to simulate various optical devices and investigate their basic characteristics.
• The experimental result obtained for multi-component PhC structures based on grooved Silicon and thermally grown oxide proves that fabrication of interference filters with almost 100 % transmission and flat-top characteristic over a selected wide range of the infrared spectrum is practical.

• For tunable LC photonic crystal filters the new design of a whole system of micro-fluidic channels and infiltration reservoirs has been developed.

• The new technique for manual infiltration of the micro-scale structures with liquid crystal has been experimentally developed.

• The fiber-optic test set-up based on end-fire technique for NIR characterization of planar integrated photonic devices has been designed and assembled.

• The mathematical approach based on transfer matrix method and random number generator in MathCad Software has been developed for simulations of the photonic band gap deviations caused by various structural deviations after fabrication process and can be used for determination of the fabrication tolerances and their compensation.

**Future work:**

From the results obtained on the relationship between TBs and angle of incidence of light for multi-component PhC structure it has become clear that even one-dimensional photonic crystal structure can be used as a broadband polarizing beam splitter in a wide-angular range. However, there is still a lot to be learnt about polarized regions of transparency:

• How the angular field of polarization splitting can be extended using the multi-component model.

• Why only the TM(H)-polarized regions of transparency possess the omnidirectional properties, while the TE(E)-polarized regions of transparency are almost totally suppressed at oblique incidence of light.

Demonstrated in this work model of fine-tunable individual channels in coupled-cavity photonic crystals have resulted in the development of the design and fabrication technology of the integrated triple channel photonic crystal filters on SOI platform. The preliminary results obtained for the first prototype structures have been included in the Chapter 4, demonstrating the modern technological capability of fabrication of this type of device. The final, improved design of the filters is currently going through the final
fabrication step at Tyndall National Institute. Similar experimental methodology to the one developed for single-cavity photonic crystals will be used for optical characterization of the device during the operation.
Appendix I

A MathCad program code for simulation of the gap map of transmission regions in 1D multi-component photonic crystal:

\[
\lambda_i := \text{SiO}_2(\phi) \\
\phi := \phi_{\text{real}} \quad i := \sqrt{-1} \\
\lambda := \text{SiO}_2(\phi) \\
U := \frac{10000}{\lambda} \\
N_t := \text{SiO}_2(\phi) \\
\lambda_s := \text{SiO}_2(\phi) \\
m := 2 \cdot \text{length}(\lambda_i) - 1 \\
N_{\lambda_i} := N_t - \lambda_s \cdot m \\
A_1 := 4 \\
\text{per} := 3 \quad N_\theta := 1 \\
N_s := 1 \quad N_L := 1 \quad Dt := 0 \\
N_t := 1.5 \quad D\theta := 0 \\
dD\theta := 0.01 \quad \text{maxt} = 16$

\[
\text{rad} = \frac{\pi}{180} \\
\text{SiO}_2 := \text{READPRN}('\text{SiO}_2\text{nl}2000.csv') \\
X_i := \text{SiO}_2 \\
\text{tr} := (t) \quad i := y = i \\
\text{Nt} := \text{SiO}_2 < 1 \\
\text{kt} := \text{SiO}_2 < 2 \\
2.. \quad \text{lengt}X \\
\text{Nkl} := \text{Nl} - k_l \cdot m \\
A := 4 \\
\text{per} := 3 \\
N_\theta := 1 \\
N_s := 1 \quad N_L := 1 \quad Dt := 0 \\
N_t := 1.5 \quad D\theta := 0 \\
dD\theta := 0.01 \quad \text{maxt} = 16$

154
$$n := 1..\text{max}$$

$$\text{DH}_1(n) := [\text{DH}_1 + d\text{DH}(n-1)]$$
$$\text{DH}_2(n) := [\text{DH}_1 + d\text{DH}(n-1)] + 2D$$

$$\text{DL}(n) := A - \text{DH}_2(n)$$

$$\text{DA}(n) := \frac{\text{DH}_1(n)}{A}$$

---

**2x2 matrix method:**

$$q_0 := \cos(\phi)$$

$$q_{10} := \sqrt{1 - \frac{(N_0)^2}{(N_k m)^2} (1 - q_0^2)}$$

$$r_{0m} := \frac{N_k m q_0 - N_0 q_{10} m}{N_k m q_0 + N_0 q_{10} m}$$

$$r_{m0} := \frac{N_0 q_0 - N_k m q_{10} m}{N_0 q_0 + N_k m q_{10} m}$$

$$Z_{0m} := N_k m q_0 + N_0 q_{10} m$$

$$Z_{m0} := N_0 q_0 + N_k m q_{10} m$$

$$t_{0m} := \frac{2 N_0 q_0}{Z_{0m}}$$

$$t_{m0} := \frac{C_{01}}{Z_{m0}}$$

$$\text{CO}_1 := 2 \cdot N_0 \cdot q_0$$
\[10q(m) := \begin{pmatrix} 1 & r0tp_m \\ r0tp_m & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t0tp_m \end{pmatrix}\]

\[10s(m) := \begin{pmatrix} 1 & r0ts_m \\ r0ts_m & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t0ts_m \end{pmatrix}\]

\[\beta(m) := 2 - \frac{\pi}{\lambda_m} \Delta t\ q0t_m\ Nkt_m\ i\]

\[\beta_t := 2 - \frac{\pi}{\lambda_m} \Delta t\ q0t_m\ Nkt_m\ i\]

\[M_t(m) := \begin{pmatrix} \beta_t(m) & 0 \\ 0 & e^{-\beta_t(m)} \end{pmatrix}\]

\[\begin{align*}
qH_m & := \sqrt{1 - \frac{(Nkt_m - q0t_m)^2}{(NH_m)^2} \left[1 - (q0t_m)^2\right]} \\
rtHp_m & := \frac{NH\ q0t_m - Nkt_m\ qH_m}{NH\ q0t_m + Nkt_m\ qH_m} \\
rtHs_m & := \frac{Nkt_m\ q0t_m - NH\ qH_m}{Nkt_m\ q0t_m + NH\ qH_m} \\
CtH_m & := \frac{2\ Nkt_m\ q0t_m}{Z\ qH_m}\ \\
CtH_m & := \frac{2\ Nkt_m\ q0t_m}{Z\ qH_m}\ \\
\end{align*}\]

\[\begin{align*}
Z4H_m := Nkt_m\ q0t_m + NH\ qH_m \\
Z4H_m := NH\ q0t_m + Nkt_m\ qH_m
\end{align*}\]

\[tHp := \frac{2\ Nkt_m\ q0t_m}{Z\ qH_m}\]

\[tHs := \frac{CtH_m}{Z\ qH_m}\]

\[\begin{align*}
ltH(m) & := \begin{pmatrix} 1 \\ rtHp_m \end{pmatrix} \begin{pmatrix} 1 \\ tHp_m \end{pmatrix} \\
ltH(m) & := \begin{pmatrix} 1 \\ rtH_m \end{pmatrix} \begin{pmatrix} 1 \\ tH_s \end{pmatrix}
\end{align*}\]

\[\beta_H(n,m) := 2 - \frac{\pi}{\lambda_m} \Delta H(n)\ qH_m\ \cdot\ NH - i\]
\[ MH(n,m) := \begin{pmatrix}
    e^{B(n,m)} & 0 \\
    0 & e^{-B(n,m)}
\end{pmatrix} \]

\[ q_{Ht} := \sqrt{1 - \frac{(NH)^2}{(N_k)_m^2} \left[ 1 - (q_{Ht})^2 \right]} \]

\[ r_{Ht} := \frac{N_k q_{Ht} - NH q_{Ht}}{N_k q_{Ht} + NH q_{Ht}} \]

\[ r_{Ht} := \frac{NH q_{Ht} - N_k q_{Ht}}{NH q_{Ht} + N_k q_{Ht}} \]

\[ Z_{Ht} := NH q_{Ht} + N_k q_{Ht} \]

\[ t_{Ht} := 2 \frac{NH q_{Ht}}{Z_{Ht}} \]

\[ C_{Ht} := 2 \times N_l q_{Ht} \]

\[ t_{Ht} := \frac{C_{Ht}}{Z_{Ht}} \]

\[ l_{Ht}(m) := \frac{1}{r_{Ht} m} \]

\[ l_{Ht}(m) := \frac{1}{r_{Ht} m} \]

\[ q_{L} := \sqrt{1 - \frac{(N_k)_m^2}{(NL)_L^2} \left[ 1 - (q_{L})^2 \right]} \]

\[ r_{L} := \frac{NL q_{Ht} - N_k q_{L}}{NL q_{Ht} + N_k q_{L}} \]

\[ r_{L} := \frac{NL q_{Ht} - N_k q_{L}}{NL q_{Ht} + N_k q_{L}} \]

\[ Z_{L} := NL q_{Ht} + N_k q_{L} \]

\[ Z_{L} := NL q_{Ht} + N_k q_{L} \]

\[ t_{L} := \frac{2 N_k q_{Ht}}{Z_{L}} \]

\[ C_{L} := 2 N_k q_{Ht} \]
$$\texttt{rt}_m := \frac{\texttt{Ct}_m}{Z\texttt{t}_m}$$

$$\texttt{ItL}_p(m) := \left(\begin{array}{cc} 1 & \texttt{rtL}_p(m) \\ \texttt{rtL}_p(m) & 1 \end{array}\right) \left(\begin{array}{c} 1 \\ \texttt{ItL}_p(m) \end{array}\right)$$

$$\texttt{ItL}_s(m) := \left(\begin{array}{cc} 1 & \texttt{rtL}_s(m) \\ \texttt{rtL}_s(m) & 1 \end{array}\right) \left(\begin{array}{c} 1 \\ \texttt{ItL}_s(m) \end{array}\right)$$

$$\beta(n,m) := \frac{2\pi}{\lambda_m} 1_{\texttt{dtL}_n(m)} q_{\texttt{tL}_m} 1_{\texttt{tL}_n(m)}$$

$$\texttt{ML}(n,m) := \left(\begin{array}{cc} \beta(n,m) & 0 \\ 0 & e^{-\beta(n,m)} \end{array}\right)$$

$$q_{\texttt{tL}_m} := \sqrt{\frac{1 - (NL)^2}{(Nk_m^2)(1 - (qtL_m)^2)}}$$

$$\texttt{rlL}_p(m) := \frac{Nk_m q_{\texttt{tL}_m} - NL q_{\texttt{tL}_m}}{Nk_m q_{\texttt{tL}_m} + NL q_{\texttt{tL}_m}}$$

$$\texttt{rlL}_s(m) := \frac{NL q_{\texttt{tL}_m} - Nk_m q_{\texttt{tL}_m}}{NL q_{\texttt{tL}_m} + Nk_m q_{\texttt{tL}_m}}$$

$$z_{\texttt{tL}_m} := Nk_m q_{\texttt{tL}_m} + NL q_{\texttt{tL}_m}$$

$$Z_{\texttt{tL}_m} := NL q_{\texttt{tL}_m} + Nk_m q_{\texttt{tL}_m}$$

$$t_{\texttt{tL}_m} := \frac{2NL q_{\texttt{tL}_m}}{Z_{\texttt{tL}_m}}$$

$$\texttt{Ct}_m := 2NL q_{\texttt{tL}_m}$$

$$\texttt{ItL}_p(m) := \left(\begin{array}{cc} 1 & \texttt{rlL}_p(m) \\ \texttt{rlL}_p(m) & 1 \end{array}\right) \left(\begin{array}{c} 1 \\ \texttt{ItL}_p(m) \end{array}\right)$$

$$\texttt{ItL}_s(m) := \left(\begin{array}{cc} 1 & \texttt{rlL}_s(m) \\ \texttt{rlL}_s(m) & 1 \end{array}\right) \left(\begin{array}{c} 1 \\ \texttt{ItL}_s(m) \end{array}\right)$$

$$q_{\texttt{tL}_m} := \sqrt{\frac{(Nk_m^2)(1 - (qtL_m)^2)}{(Nt)^2}}$$

$$\texttt{rtL}_m := \frac{Ns q_{\texttt{tL}_m} - Nk_m q_{\texttt{tL}_m}}{Ns q_{\texttt{tL}_m} + Nk_m q_{\texttt{tL}_m}}$$

$$\texttt{Ct}_m := 2NL q_{\texttt{tL}_m}$$
\[
\begin{align*}
rtLasts_m & := Nk_m qHt_m - Ns qLast_m \\
ZtLastp_m & := Ns qHt_m + Nk_m qLast_m \\
ZtLasts_m & := Nk_m qHt_m + Ns qLast_m \\
tlLastp_m & = \frac{2 Nk_m qHt_m}{ZtLastp_m} \\
tlLasts_m & = \frac{2 Nk_m qHt_m}{ZtLasts_m} \\
CtLast_m & := 2 NL - qLt_m \\
litLastp(m) & := \left( \frac{1}{rtLastp_m} \right) \left( \frac{1}{tlLastp_m} \right) \\
litLasts(m) & := \left( \frac{1}{rtLasts_m} \right) \left( \frac{1}{tlLasts_m} \right) \\
sp(n, m) & := (IHt(m) - Mt(m) - tLp(m) - ML(n, m) - LLp(m) - Mt(m) - tHgtm - MH(n, m))^T \\
ss(n, m) & := (IHt^m - Mt(m) - tLts(m) - ML(n, m) - LLts(m) - Mt(m) - tHgtm - MH(n, m))^T \\
Sp(n, m) & := tLp(m) - Mt(m) - tHgtm - MH(n, m) - sp(n, m) - IHt(m) - Mt(m) - tLasts(m) \\
Ss(n, m) & := tLts(m) - Mt(m) - tHt(m) - Mt(m) - sLs(n, m) - IHt^m - Mt^m - tLasts(m) \\
n(n, m) & := \left( \frac{(Ss(n, m))_{1,0}}{(Ss(n, m))_{0,0}} \right)^2 \\
rp(n, m) & := \left( \frac{(Sp(n, m))_{1,0}}{(Sp(n, m))_{0,0}} \right)^2 \\
sp(n, m) & := \frac{Nk}{N} \left[ \left( \frac{1}{Sp(n, m)} \right)_{0,0} \right]^2 \\
tp(n, m) & := \frac{Ns}{N} \left[ \left( \frac{1}{Sp(n, m)} \right)_{0,0} \right]^2 \\
ts(n, m) & := \frac{Nk}{N} \left[ \left( \frac{1}{Ss(n, m)} \right)_{0,0} \right]^2
\end{align*}
\]

cutoff level - Tpbg

\[
M^{(\lambda)} := \begin{pmatrix} \lambda \end{pmatrix}, \quad M^{(\gamma)} := \begin{pmatrix} \gamma \end{pmatrix}, \quad M^{(\varphi)} := \begin{pmatrix} \varphi \end{pmatrix}
\]

159
\[ T_{\text{bg}} := 0.95 \]
\[ t_{p1}^{n,m} := t_p(n,m) \]
\[ t_{s1}^{n,m} := t_s(n,m) \]
\[ q_{pl}^{n,m} := \text{if}\left(t_{p1}^{n,m} > T_{\text{bg}}, t_{p1}^{n,m}, 0\right) \]
\[ q_{pl}^{n,m} := q_{pl}(n,m) \]
\[ q_{sl}^{n,m} := \text{if}\left(t_{s1}^{n,m} > T_{\text{bg}}, t_{s1}^{n,m}, 0\right) \]
\[ q_{sl}^{n,m} := q_{sl}(n,m) \]
\[ w_{pl}^{n,m} := w_{pl}(n,m) \]
\[ d_{qpl}^{n,m} := \text{if}\left(t_{p1}^{n,m} \geq T_{\text{bg}} \land t_{p1}^{n,m-2} \geq T_{\text{bg}} \land t_{p1}^{n,m-1} \geq T_{\text{bg}} \land t_{p1}^{n,m} \geq T_{\text{bg}} \right) \]
\[ d_{qpl}^{n,m} := d_{qpl}(n,m) \]

**BEFORE CUTOFF PROCESS:**

[Graphs showing data]
After CUTOFF Process:

FILLING FRACTION, as a function of DH and Wavelength

\[ DA(n, m) := \frac{\text{dqpl}_{n, m}}{\text{tp}_{n, m}} \]

NORMALIZED FREQUENCY, WAVENUMBER, CM\(^{-1}\)

\[ \lambda_{\text{m}} \]

\[ w_{\text{p}, n, m} \]

161
Appendix II

A MathCad program code for simulation of the reflection spectra and gap maps of 1D photonic crystal with triple-cavity.

\[ i := \sqrt{-1} \]
\[ \phi := 0 \]
\[ \Delta \lambda := 0.0001 \]
\[ m := 1 \ldots 6000 \]
\[ \lambda_0 := 1.2 \]
\[ \lambda_m := \lambda_0 + \Delta \lambda \cdot (m - 1) \quad m := \frac{10000}{\lambda_m} \]

\[ A1 := 0.8 \]
\[ \text{perl} := 2 \]
\[ \text{per2} := 2 \]
\[ N0 := 1.0 \]
\[ Ns := 1 \]
\[ NH := 3.42 \]
\[ NL := 1 \]
\[ \text{maxn} := 10 \]
\[ n := 1 \ldots \text{maxn} \]
\[ d\text{DH} := 0.001 \]
\[ \text{DH0} := 0.368 \]

\[ \text{DH1}(n) := \text{DH0} + d\text{DH}(n - 1) \]
\[ \text{DL1}(n) := A1 - \text{DH1}(n) \]
\[ \text{DA1}(n) := \frac{\text{DH1}(n)}{A1} \]
Ddef(n) := DL1(n)

Defect refractive index

k := 1..100

Ndef1(k) := 1.54 + (k - 1)0.00

Ndef3(k) := 1.54 - (k - 1)0.002

Ndef2(k) := 1.54 - (k - 1)0.00

2x2matrix method:

rad := \frac{\pi}{180}

\phi := \phi \cdot rad

q0 := \cos(\phi)

q0H := \sqrt{1 - \frac{(No)^2}{(NH)^2} \cdot (1 - q0^2)}

r0lp := \frac{NH \cdot q0 - No \cdot q0H}{NH \cdot q0 + No \cdot q0H}

r0ls := \frac{No \cdot q0 - NH \cdot q0H}{No \cdot q0 + NH \cdot q0H}

t0lp := 2 \cdot No \cdot \frac{q0}{NH \cdot q0 + No \cdot q0H}

r0ls := \frac{No \cdot q0 - NH \cdot q0H}{No \cdot q0 + NH \cdot q0H}

t0ls := 2 \cdot No \cdot \frac{q0}{No \cdot q0 + NH \cdot q0H}

I01s := \begin{pmatrix} 1 & r01s \\ r01s & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t01s \end{pmatrix}

I01p := \begin{pmatrix} 1 & r01p \\ r01p & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t01p \end{pmatrix}
\[ \beta_{n,m} := \frac{2 \pi}{\lambda_m} \cdot \text{DH}_l(n) \cdot \text{qO}H \cdot \text{NH} \cdot \text{i} \]

\[ \text{LH}_l(n,m) := \begin{pmatrix} e^{\beta_{n,m}} & 0 \\ 0 & e^{-\beta_{n,m}} \end{pmatrix} \]

\[ \text{qHL} := \sqrt{1 - \frac{(\text{NH})^2}{(\text{NL})^2} \left[ 1 - (\text{qO}H)^2 \right]} \]

\[ \text{rHL}_p := \frac{\text{NL} \cdot \text{qO}H - \text{NH} \cdot \text{qHL}}{\text{NL} \cdot \text{qO}H + \text{NH} \cdot \text{qHL}} \]

\[ \text{tHL}_p := 2 \cdot \text{NH} \cdot \frac{\text{qO}H}{\text{NL} \cdot \text{qO}H + \text{NH} \cdot \text{qHL}} \]

\[ \text{IHL}_p := \frac{1}{\text{rHL}_p} \left( \frac{1}{\text{tHL}_p} \right) \]

\[ \text{qLH} := \sqrt{1 - \frac{(\text{NL})^2}{(\text{NH})^2} \left[ 1 - (\text{qHL})^2 \right]} \]

\[ \text{rLH}_p := \frac{\text{NH} \cdot \text{qHL} - \text{NL} \cdot \text{qLH}}{\text{NH} \cdot \text{qHL} + \text{NL} \cdot \text{qLH}} \]

\[ \text{tLH}_p := 2 \cdot \text{NL} \cdot \frac{\text{qHL}}{\text{NL} \cdot \text{qHL} + \text{NH} \cdot \text{qLH}} \]

\[ \text{IHL}_p := \frac{1}{\text{rLH}_p} \left( \frac{1}{\text{tLH}_p} \right) \]

\[ \beta_{n,m} := \frac{2 \pi}{\lambda_m} \cdot \text{DH}_l(n) \cdot \text{qL}H \cdot \text{NH} \cdot \text{i} \]

\[ \text{LH}(n,m) := \begin{pmatrix} e^{\beta_{n,m}} & 0 \\ 0 & e^{-\beta_{n,m}} \end{pmatrix} \]
\[ q_{\text{odo Defl}}(k) := \sqrt{1 - \frac{(NH)^2}{(N_{\text{defl}}(k))^2} \left[ 1 - (q_{LH})^2 \right]} \]

\[ r_{\text{Hdo Defs l}}(k) := \frac{NH - q_{LH} - N_{\text{defl}}(k) \cdot q_{\text{odo Defl}}(k)}{NH - q_{LH} + N_{\text{defl}}(k) \cdot q_{\text{odo Defl}}(k)} \]

\[ r_{\text{Hdo Defp l}}(k) := \frac{N_{\text{defl}}(k) \cdot q_{LH} - NH - q_{\text{odo Defl}}(k)}{N_{\text{defl}}(k) \cdot q_{LH} + NH - q_{\text{odo Defl}}(k)} \]

\[ t_{\text{Hdo Defs l}}(k) := 2 \cdot NH \frac{q_{LH}}{NH \cdot q_{LH} + N_{\text{defl}}(k) \cdot q_{\text{odo Defl}}(k)} \]

\[ t_{\text{Hdo Defp l}}(k) := 2 \cdot NH \frac{q_{LH}}{N_{\text{defl}}(k) \cdot q_{LH} + NH \cdot q_{\text{odo Defl}}(k)} \]

\[ I_{\text{Hdo Defp l}}(k) := \begin{pmatrix} 1 & r_{\text{Hdo Defp l}}(k) \\ r_{\text{Hdo Defp l}}(k) & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t_{\text{Hdo Defp l}}(k) \end{pmatrix} \]

\[ \beta_{\text{defl}}(n, m, k) := 2 \cdot \frac{\pi}{\lambda_m} \cdot D_{\text{defl}}(n) \cdot q_{\text{odo Defl}}(k) \cdot N_{\text{defl}}(k) \cdot i \]

\[ I_{\text{Hdo Defs l}}(k) := \begin{pmatrix} 1 & r_{\text{Hdo Defs l}}(k) \\ r_{\text{Hdo Defs l}}(k) & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t_{\text{Hdo Defs l}}(k) \end{pmatrix} \]

\[ L_{\text{defl}}(n, m, k) := \begin{pmatrix} e^{\beta_{\text{defl}}(n, m, k)} & 0 \\ 0 & e^{-\beta_{\text{defl}}(n, m, k)} \end{pmatrix} \]

\[ q_{\text{posle Def l}}(k) := \sqrt{1 - \frac{(N_{\text{defl}}(k))^2}{(NH)^2} \left[ 1 - (q_{\text{odo Defl}}(k))^2 \right]} \]

\[ r_{\text{DefH p l}}(k) := \frac{NH - q_{\text{odo Defl}}(k) - N_{\text{defl}}(k) \cdot q_{\text{posle Def l}}(k)}{NH - q_{\text{odo Defl}}(k) + N_{\text{defl}}(k) \cdot q_{\text{posle Def l}}(k)} \]
\[ t_{\text{DefHp}}(k) := 2 \cdot N_{\text{def}}(k) \cdot \frac{q_{\text{doDef}}(k)}{N_{\text{def}}(k) \cdot q_{\text{doDef}}(k) + NH \cdot q_{\text{posleDef}}(k)} \]

\[ l_{\text{DefHp}}(k) := \frac{1}{r_{\text{DefHp}}(k)} \cdot \left( \frac{1}{t_{\text{DefHp}}(k)} \right) \]

\[ r_{\text{DefHs}}(k) := \frac{N_{\text{def}}(k) \cdot q_{\text{doDef}}(k) - NH \cdot q_{\text{posleDef}}(k)}{N_{\text{def}}(k) \cdot q_{\text{doDef}}(k) + NH \cdot q_{\text{posleDef}}(k)} \]

\[ t_{\text{DefHs}}(k) := 2 \cdot N_{\text{def}}(k) \cdot \frac{q_{\text{doDef}}(k)}{N_{\text{def}}(k) \cdot q_{\text{doDef}}(k) + NH \cdot q_{\text{posleDef}}(k)} \]

\[ l_{\text{DefHs}}(k) := \frac{1}{r_{\text{DefHs}}(k)} \cdot \left( \frac{1}{t_{\text{DefHs}}(k)} \right) \]

\[ q_{\text{doDef2}}(k) := \sqrt{1 - \frac{(NH)^2}{(N_{\text{def2}}(k))^2 \left[1 - (q LH)^2 \right]}} \]

\[ r_{\text{HdoDefp}}z(k) := \frac{N_{\text{def2}}(k) \cdot q LH - NH \cdot q_{\text{doDef2}}(k)}{N_{\text{def2}}(k) \cdot q LH + NH \cdot q_{\text{doDef2}}(k)} \]

\[ r_{\text{HdoDefs}}z(k) := \frac{NH \cdot q LH - N_{\text{def2}}(k) \cdot q_{\text{doDef2}}(k)}{NH \cdot q LH + N_{\text{def2}}(k) \cdot q_{\text{doDef2}}(k)} \]

\[ t_{\text{HdoDefs}}z(k) := 2 \cdot NH \cdot \frac{q LH}{NH \cdot q LH + N_{\text{def2}}(k) \cdot q_{\text{doDef2}}(k)} \]

\[ t_{\text{HdoDefp}}z(k) := 2 \cdot NH \cdot \frac{q LH}{N_{\text{def2}}(k) \cdot q LH + NH \cdot q_{\text{doDef2}}(k)} \]

\[ l_{\text{HdoDefp}}z(k) := \frac{1}{r_{\text{HdoDefp}}z(k)} \cdot \left( \frac{1}{t_{\text{HdoDefp}}z(k)} \right) \]

\[ l_{\text{HdoDefs}}z(k) := \frac{1}{r_{\text{HdoDefs}}z(k)} \cdot \left( \frac{1}{t_{\text{HdoDefs}}z(k)} \right) \]

167
\[ \beta_{\text{def}2}(n, m, k) := 2 \cdot \frac{\pi}{\lambda m} \cdot \text{Ddef}(n) \cdot \text{qdoDef}2(k) \cdot \text{Ndef}2(k) \cdot i \]

\[ \text{Ldef}2(n, m, k) := \begin{pmatrix} e^{\beta_{\text{def}2}(n, m, k)} & 0 \\ 0 & e^{-\beta_{\text{def}2}(n, m, k)} \end{pmatrix} \]

\[ \text{qposleDef}^2(k) := \sqrt{1 - \frac{(\text{Ndef}2(k))^2}{(\text{NH})^2} \left[ 1 - (\text{qdoDef}2(k))^2 \right]} \]

\[ r_{\text{Def}Hp^2}(k) := \frac{\text{NH} \cdot \text{qdoDef}2(k) - \text{Ndef}2(k) \cdot \text{qposleDef}^2(k)}{\text{NH} \cdot \text{qdoDef}2(k) + \text{Ndef}2(k) \cdot \text{qposleDef}^2(k)} \]

\[ r_{\text{Def}Hs^2}(k) := \frac{\text{Ndef}2(k) \cdot \text{qdoDef}2(k) - \text{NH} \cdot \text{qposleDef}^2(k)}{\text{Ndef}2(k) \cdot \text{qdoDef}2(k) + \text{NH} \cdot \text{qposleDef}^2(k)} \]

\[ t_{\text{Def}Hp^2}(k) := \frac{2 \cdot \text{Ndef}2(k) \cdot \text{qdoDef}2(k)}{\text{Ndef}2(k) \cdot \text{qdoDef}2(k) + \text{NH} \cdot \text{qposleDef}^2(k)} \]

\[ I_{\text{Def}Hp^2}(k) := \begin{pmatrix} 1 & r_{\text{Def}Hp^2}(k) \\ r_{\text{Def}Hp^2}(k) & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t_{\text{Def}Hp^2}(k) \end{pmatrix} \]

\[ t_{\text{Def}Hs^2}(k) := \frac{2 \cdot \text{Ndef}2(k) \cdot \text{qdoDef}2(k)}{\text{Ndef}2(k) \cdot \text{qdoDef}2(k) + \text{NH} \cdot \text{qposleDef}^2(k)} \]

\[ I_{\text{Def}Hs^2}(k) := \begin{pmatrix} 1 & r_{\text{Def}Hs^2}(k) \\ r_{\text{Def}Hs^2}(k) & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t_{\text{Def}Hs^2}(k) \end{pmatrix} \]

\[ \text{qdoDef}3(k) := \sqrt{1 - \frac{(\text{NH})^2}{(\text{Ndef}3(k))^2} \left[ 1 - (\text{qLH})^2 \right]} \]

\[ r_{\text{HdoDef}3}(k) := \frac{\text{NH} \cdot \text{qLH} - \text{Ndef}3(k) \cdot \text{qdoDef}3(k)}{\text{NH} \cdot \text{qLH} + \text{Ndef}3(k) \cdot \text{qdoDef}3(k)} \]
\[ r_{HdDefs}(k) := \frac{N_{def}(k) \cdot qLH - NH \cdot qdoDef(k)}{N_{def}(k) \cdot qLH + NH \cdot qdoDef(k)} \]

\[ t_{HdDefs}(k) := 2 \cdot NH \frac{qLH}{NH \cdot qLH + N_{def}(k) \cdot qdoDef(k)} \]

\[ \beta_{def}(n, m, k) := 2 \cdot \pi \cdot D_{def}(n) \cdot qdoDef(k) \cdot N_{def}(k) \cdot i \]

\[ l_{HdDefs}(k) := \left( \begin{array}{cc} 1 & r_{HdDefs}(k) \\ r_{HdDefs}(k) & 1 \end{array} \right) \left( \begin{array}{c} 1 \\ t_{HdDefs}(k) \end{array} \right) \]

\[ l_{HdDefp}(k) := \left( \begin{array}{cc} 1 & r_{HdDefp}(k) \\ r_{HdDefp}(k) & 1 \end{array} \right) \left( \begin{array}{c} 1 \\ t_{HdDefp}(k) \end{array} \right) \]

\[ L_{def}(n, m, k) := \begin{pmatrix} e^{\beta_{def}(n, m, k)} & 0 \\ 0 & e^{-\beta_{def}(n, m, k)} \end{pmatrix} \]

\[ q_{posleDef}(k) := \sqrt{1 - \left( \frac{N_{def}(k)}{NH} \right)^2 \left[ 1 - (q_{doDef}(k))^2 \right]} \]

\[ r_{DefHp}(k) := \frac{NH \cdot q_{doDef}(k) - N_{def}(k) \cdot q_{posleDef}(k)}{NH \cdot q_{doDef}(k) + N_{def}(k) \cdot q_{posleDef}(k)} \]

\[ r_{DefHs}(k) := \frac{N_{def}(k) \cdot q_{doDef}(k) - NH \cdot q_{posleDef}(k)}{N_{def}(k) \cdot q_{doDef}(k) + NH \cdot q_{posleDef}(k)} \]

\[ t_{DefHp}(k) := 2 \cdot N_{def}(k) \cdot \frac{q_{doDef}(k)}{N_{def}(k) \cdot q_{doDef}(k) + NH \cdot q_{posleDef}(k)} \]

\[ l_{DefHp}(k) := \left( \begin{array}{cc} 1 & r_{DefHp}(k) \\ r_{DefHp}(k) & 1 \end{array} \right) \left( \begin{array}{c} 1 \\ t_{DefHp}(k) \end{array} \right) \]

169
$t_{\text{DefHs3} k} := 2 \cdot N_{\text{def3}}(k) \cdot \frac{q_{\text{doDef3}}(k)}{N_{\text{def3}}(k) \cdot q_{\text{doDef3}}(k) + NH \cdot q_{\text{posleDef3} k}}$

$I_{\text{DefHs3} k} := \left( \begin{array}{cc} 1 & r_{\text{DefHs3} k} \\ r_{\text{DefHs3} k} & 1 \end{array} \right) \cdot \left( \begin{array}{c} 1 \\ \left(t_{\text{DefHs3} k}\right) \end{array} \right)$

$q_{\text{Last}} := \sqrt{1 - \frac{(NH)^2}{(Ns)^2} \left[1 - (QLH)^2\right]}$

$r_{\text{Lasts}} := \frac{NH \cdot QLH - N_{\text{sLast}}}{NH \cdot QLH + N_{\text{sLast}}} \quad r_{\text{Lastp}} := \frac{N_{\text{sQLH}} - NH \cdot q_{\text{Last}}}{N_{\text{sQLH}} + NH \cdot q_{\text{Last}}}$

$t_{\text{Lasts}} := 2 \cdot NH \cdot \frac{QLH}{NH \cdot QLH + N_{\text{sLast}}}$

$t_{\text{Lastp}} := 2 \cdot NH \cdot \frac{QLH}{N_{\text{sQLH}} + NH \cdot q_{\text{Last}}}$

$I_{\text{Lastp}} := \left( \begin{array}{c} 1 & r_{\text{Lastp}} \\ r_{\text{Lastp}} & 1 \end{array} \right) \cdot \left( \begin{array}{c} 1 \\ \left(t_{\text{Lastp}}\right) \end{array} \right)$

$I_{\text{Lasts}} := \left( \begin{array}{cc} 1 & r_{\text{Lasts}} \\ r_{\text{Lasts}} & 1 \end{array} \right) \cdot \left( \begin{array}{c} 1 \\ \left(t_{\text{Lasts}}\right) \end{array} \right)$

$Inp(n,m,k) := 101p \cdot LH1(n,m) \cdot (IHLp \cdot LL1(n,m) \cdot ILHp \cdot LH(n,m))^1$

$Ins(n,m,k) := 101s \cdot LH1(n,m) \cdot (IHLs \cdot LL1(n,m) \cdot ILHs \cdot LH(n,m))^1$

$deflp(n,m,k) := (I\text{HdoDefp } k) \cdot L\text{defl}(n,m,k) \cdot I\text{DefHp } k \cdot LH(n,m))^1$

$Deflp(n,m,k) := deflp(n,m,k) \cdot (I\text{HLp} \cdot LL1(n,m) \cdot ILHp \cdot LH(n,m))^1$
defls(n, m, k) := (IHdoDefsl(k) · Defl(n, m, k) · IDefHsl(k) · LH(n, m))^1
Defls(n, m, k) := defls(n, m, k) · (IHLp·LLl(n, m)·ILHp·LH(n, m))^1
def2p(n, m, k) := (IHdoDefp2(k) · Def2(n, m, k) · IDefHp2(k) · LH(n, m))^1
def2s(n, m, k) := (IHdoDefss2(k) · Def2(n, m, k) · IDefHss2(k) · LH(n, m))^1
Def2p(n, m, k) := def2p(n, m, k) · (IHLp·LLl(n, m)·ILHp·LH(n, m))^1
Def2s(n, m, k) := def2s(n, m, k) · (IHLp·LLl(n, m)·ILHp·LH(n, m))^1
def3p(n, m, k) := (IHdoDefp3(k) · Def3(n, m, k) · IDefHp3(k) · LH(n, m))^1
def3s(n, m, k) := (IHdoDefss3(k) · Def3(n, m, k) · IDefHss3(k) · LH(n, m))^1
Def3p(n, m, k) := def3p(n, m, k) · (IHLp·LLl(n, m)·ILHp·LH(n, m))^1
Def3s(n, m, k) := def3s(n, m, k) · (IHLp·LLl(n, m)·ILHp·LH(n, m))^1
sp(n, m, k) := Inp(n, m, k) · Deflp(n, m, k) · DeGp(n, m, k) · DeOp(n, m, k) · ILastp
ss(n, m, k) := Ins(n, m, k) · Defls(n, m, k) · Defs(n, m, k) · Defss(n, m, k) · ILasts
rp(n, m, k) := \begin{bmatrix}
(s(n, m, k))_1, 0 \\
(s(n, m, k))_0, 0
\end{bmatrix}
\quad tp(n, m, k) := \frac{Ns}{No} \begin{bmatrix}
1 \\
(s(n, m, k))_0, 0
\end{bmatrix}^2
\quad m := \frac{10000}{\lambda_m}
\quad tfm := \frac{A1}{\lambda_m}
\quad ns(n, m, k) := \frac{Ns}{No} \begin{bmatrix}
1 \\
(s(n, m, k))_0, 0
\end{bmatrix}
\[
\frac{rp(1, m, 25)}{rp(1, m, \text{FRAME})}
\]

\[
rp(144, m, 1)
\]

\[
\frac{\text{rp}, m, 1 := \text{rp}(n, m, 1)}{10000}
\]

<table>
<thead>
<tr>
<th>( \lambda_m )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.01</td>
</tr>
<tr>
<td>0.02</td>
</tr>
<tr>
<td>0.03</td>
</tr>
<tr>
<td>0.04</td>
</tr>
<tr>
<td>0.05</td>
</tr>
<tr>
<td>0.06</td>
</tr>
<tr>
<td>0.07</td>
</tr>
<tr>
<td>0.08</td>
</tr>
<tr>
<td>0.09</td>
</tr>
</tbody>
</table>

\[
\begin{array}{ccccccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0.29335 & 0.29022 & 0.28706 & 0.28386 & 0.28062 & 0.27735 & 0.27404 & 0.27069 & 0.26734 \\
2 & 0.41936 & 0.41711 & 0.41483 & 0.41253 & 0.41019 & 0.40783 & 0.40545 & 0.40303 & 0.39955 \\
3 & 0.51814 & 0.51653 & 0.51493 & 0.51324 & 0.51157 & 0.50987 & 0.50813 & 0.50642 & 0.50459 \\
4 & 0.59631 & 0.59517 & 0.59401 & 0.59283 & 0.59164 & 0.59043 & 0.58921 & 0.58797 & 0.58672 \\
5 & 0.65872 & 0.65793 & 0.65712 & 0.65629 & 0.65546 & 0.65461 & 0.65376 & 0.65288 & 0.65198 \\
6 & 0.70898 & 0.70844 & 0.70789 & 0.70733 & 0.70676 & 0.70618 & 0.70556 & 0.70495 & 0.70435 \\
7 & 0.74976 & 0.74941 & 0.74906 & 0.7487 & 0.74833 & 0.74795 & 0.74757 & 0.74718 & 0.74678 \\
8 & 0.78311 & 0.78229 & 0.78278 & 0.78248 & 0.78227 & 0.78204 & 0.78181 & 0.78157 & 0.78132 \\
9 & 0.80558 & 0.80464 & 0.80373 & 0.80289 & 0.80206 & 0.80124 & 0.80040 & 0.79956 & 0.79871 \\
10 & 0.83329 & 0.83329 & 0.83329 & 0.83329 & 0.83329 & 0.83329 & 0.83329 & 0.83329 & 0.83329 \\
\end{array}
\]

172
A MathCad program code for simulation of the reflection spectra and gap maps of 1D photonic crystal with structural deviations.

\[
\begin{align*}
\lambda_0 & := 1 \\
\mathbf{m} & := 1 \ldots 2000 \quad \delta \lambda := 0.01 \quad i := \sqrt{-1} \\
N_s & := 1 \\
N_0 & := 1 \\
N_H & := 3.42 \\
N_L & := 1 \\
N_{\text{def}} & := 1 \\
\text{maxn} & := 100 \\
n & := 1 \ldots \text{maxn}
\end{align*}
\]

\[
\begin{align*}
d_{DH} & := \frac{\text{LatCon}}{\text{maxn}} \\
D_H & := 0 \\
D_H(n) & := D_H + d_{DH}(n - 1) \\
D_{L1}(n) & := \text{LatCon} - D_H(n) \\
D_A(n) & := \frac{D_H(n)}{\text{LatCon}} \\
s_1 & := 8 \\
\mu_1 & := 0.1 \\
\sigma_1 & := 0.1 \\
\text{bin} & := 50
\end{align*}
\]
\[ N := \text{rnorm}(s1, \mu, \sigma) \]

\[
\text{upper} := \text{ceil}(\text{max}(N)) \\
\text{lower} := \text{floor}(\text{min}(N)) \\
j := 0..\text{bin} \\
h := \frac{\text{upper} - \text{lower}}{\text{bin}} \\
\text{int}_j := \text{lower} + h \cdot j \\
\text{int} := \text{int} + 0.5 \cdot h \\
f := \text{hist}(\text{int}, N) \\
\mathcal{F}(x) := s \cdot h \cdot \text{dnorm}(x, \mu, \sigma) \]

Normal fitting function:

\[ h := 0..8-1 \]

\[
\begin{array}{c}
\text{Histogram} \\
\text{Normal fit} \\
\end{array}
\]

\[ s := 8 \]

\[ \mu := 0 \]

\[ \sigma_H := 0.05 \]
\[ \text{DisOrd} := \frac{\sigma_H}{\text{LatCon}} \]

\[ \text{DisOrd} 100 = 1.667 \]

\[ \dd H_{h,n} := DH(n) \cdot dDH_h \]

\[ \begin{align*}
\text{DH1}(n) & := DH(n) + \dd H_{0,n} \\
\text{DH2}(n) & := DH(n) + \dd H_{1,n} \\
\text{DH3}(n) & := DH(n) + \dd H_{2,n} \\
\text{DH4}(n) & := DH(n) + \dd H_{3,n} \\
\text{DH5}(n) & := DH(n) + \dd H_{4,n} \\
\text{DH6}(n) & := DH(n) + \dd H_{5,n} \\
\text{DH7}(n) & := DH(n) + \dd H_{6,n} \\
\text{DH8}(n) & := DH(n) + \dd H_{7,n}
\end{align*} \]
DL12(n) := \text{LatCon} - \frac{DH1(n) + DH2(n)}{2}

DL34(n) := \text{LatCon} - \frac{DH3(n) + DH4(n)}{2}

DL56(n) := \text{LatCon} - \frac{DH5(n) + DH6(n)}{2}

DL78(n) := \text{LatCon} - \frac{DH7(n) + DH8(n)}{2}

DL23(n) := \text{LatCon} - \frac{DH2(n) + DH3(n)}{2}

DL45(n) := \text{LatCon} - \frac{DH4(n) + DH5(n)}{2}

DL67(n) := \text{LatCon} - \frac{DH6(n) + DH7(n)}{2}

I01 := \begin{pmatrix} 1 & r01 \\ r01 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t01 \end{pmatrix}

r01 := \frac{NH - No}{NH + No} \quad t01 := 2 \cdot \frac{No \cdot 1}{NH + No}

\beta H1(n, m) := 2 \cdot \pi \cdot \lambda_m \cdot DH1(n) \cdot NH \cdot i

LH1(n, m) := \begin{pmatrix} e^{\beta H1(n, m)} & 0 \\ 0 & e^{-\beta H1(n, m)} \end{pmatrix}
\[
\begin{align*}
t_{HL} &:= 2 \cdot NH \cdot \frac{1}{NL + NH} \\
I_{HL} &:= \left(\frac{1}{r_{HL}}, \frac{1}{t_{HL}}\right) \\
\beta_{L12} (n, m) &:= 2 \cdot \frac{\pi}{\lambda_m} \cdot DL_{12}(n) \cdot NL \cdot i \\
L_{12}(n, m) &:= \begin{pmatrix} e^{\beta_{L12} (n, m)} & 0 \\ 0 & e^{-\beta_{L12} (n, m)} \end{pmatrix} \\
r_{LH} &:= \frac{(NH - NL)}{(NH + NL)} \\
t_{LH} &:= 2 \cdot NL \cdot \frac{1}{NH + NL} \\
I_{LH} &:= \left(\frac{1}{r_{LH}}, \frac{1}{t_{LH}}\right) \\
\beta_{H2} (n, m) &:= 2 \cdot \frac{\pi}{\lambda_m} \cdot DH_{2}(n) \cdot NH \cdot i \\
\beta_{L23} (n, m) &:= 2 \cdot \frac{\pi}{\lambda_m} \cdot DL_{23}(n) \cdot NL \cdot i \\
\beta_{H3} (n, m) &:= 2 \cdot \frac{\pi}{\lambda_m} \cdot DH_{3}(n) \cdot NH \cdot i \\
\beta_{L34} (n, m) &:= 2 \cdot \frac{\pi}{\lambda_m} \cdot DL_{34}(n) \cdot NL \cdot i \\
L_{H2}(n, m) &:= \begin{pmatrix} e^{\beta_{H2} (n, m)} & 0 \\ 0 & e^{-\beta_{H2} (n, m)} \end{pmatrix}
\end{align*}
\]
\[
L_{23}(n,m) := \begin{pmatrix}
  e^\beta L_{23}(n,m) & 0 \\
  0 & e^{-\beta L_{23}(n,m)}
\end{pmatrix}
\]

\[
L_{H3}(n,m) := \begin{pmatrix}
  e^\beta H_{3}(n,m) & 0 \\
  0 & e^{-\beta H_{3}(n,m)}
\end{pmatrix}
\]

\[
L_{34}(n,m) := \begin{pmatrix}
  e^\beta L_{34}(n,m) & 0 \\
  0 & e^{-\beta L_{34}(n,m)}
\end{pmatrix}
\]

\[
\beta H_{4}(n,m) := 2 \cdot \frac{\pi}{\lambda} \cdot D_{H4(n)} \cdot N_{H} \cdot i
\]

\[
\beta L_{45}(n,m) := 2 \cdot \frac{\pi}{\lambda} \cdot D_{L45(n)} \cdot N_{L} \cdot i
\]

\[
\beta H_{5}(n,m) := 2 \cdot \frac{\pi}{\lambda} \cdot D_{H5(n)} \cdot N_{H} \cdot i
\]

\[
\beta L_{56}(n,m) := 2 \cdot \frac{\pi}{\lambda} \cdot D_{L56(n)} \cdot N_{L} \cdot i
\]

\[
L_{H4}(n,m) := \begin{pmatrix}
  e^\beta H_{4}(n,m) & 0 \\
  0 & e^{-\beta H_{4}(n,m)}
\end{pmatrix}
\]

\[
L_{45}(n,m) := \begin{pmatrix}
  e^\beta L_{45}(n,m) & 0 \\
  0 & e^{-\beta L_{45}(n,m)}
\end{pmatrix}
\]

\[
L_{H5}(n,m) := \begin{pmatrix}
  e^\beta H_{5}(n,m) & 0 \\
  0 & e^{-\beta H_{5}(n,m)}
\end{pmatrix}
\]

\[
L_{56}(n,m) := \begin{pmatrix}
  e^\beta L_{56}(n,m) & 0 \\
  0 & e^{-\beta L_{56}(n,m)}
\end{pmatrix}
\]
\[
\beta H_6(n,m) := 2 \cdot \frac{\pi}{\lambda_m} \cdot DH_6(n) \cdot NH_i
\]

\[
\beta L_{67}(n,m) := 2 \cdot \frac{\pi}{\lambda_m} \cdot DL_{67}(n) \cdot NL_i
\]

\[
\beta H_7(n,m) := 2 \cdot \frac{\pi}{\lambda_m} \cdot DH_7(n) \cdot NH_i
\]

\[
\beta L_{78}(n,m) := 2 \cdot \frac{\pi}{\lambda_m} \cdot DL_{78}(n) \cdot NL_i
\]

\[
\beta H_8(n,m) := 2 \cdot \frac{\pi}{\lambda_m} \cdot DH_8(n) \cdot NH_i
\]

\[
LH_6(n,m) := \begin{pmatrix}
 e^{\beta H_6(n,m)} & 0 \\
0 & e^{-\beta H_6(n,m)}
\end{pmatrix}
\]

\[
L_{67}(n,m) := \begin{pmatrix}
 e^{\beta L_{67}(n,m)} & 0 \\
0 & e^{-\beta L_{67}(n,m)}
\end{pmatrix}
\]

\[
LH_7(n,m) := \begin{pmatrix}
 e^{\beta H_7(n,m)} & 0 \\
0 & e^{-\beta H_7(n,m)}
\end{pmatrix}
\]

\[
L_{78}(n,m) := \begin{pmatrix}
 e^{\beta L_{78}(n,m)} & 0 \\
0 & e^{-\beta L_{78}(n,m)}
\end{pmatrix}
\]

\[
LH_8(n,m) := \begin{pmatrix}
 e^{\beta H_8(n,m)} & 0 \\
0 & e^{-\beta H_8(n,m)}
\end{pmatrix}
\]
\[ r_{last} := \frac{Ns - NH}{Ns + NH} \quad t_{last} := 2 \cdot NH \cdot \frac{1}{NH + Ns} \]

\[ \begin{pmatrix} 1 & r_{last} \\ r_{last} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ t_{last} \end{pmatrix} \]

\[ P_1(n,m) := LH1(n,m) \cdot IHL \cdot L12(n,m) \cdot ILH \]
\[ P_2(n,m) := LH2(n,m) \cdot IHL \cdot L23(n,m) \cdot ILH \]
\[ P_3(n,m) := LH3(n,m) \cdot IHL \cdot L34(n,m) \cdot ILH \]
\[ P_4(n,m) := LH4(n,m) \cdot IHL \cdot L45(n,m) \cdot ILH \]
\[ P_5(n,m) := LH5(n,m) \cdot IHL \cdot L56(n,m) \cdot IL \]
\[ P_6(n,m) := LH6(n,m) \cdot IHL \cdot L67(n,m) \cdot ILH \]
\[ P_7(n,m) := LH7(n,m) \cdot IHL \cdot L78(n,m) \cdot ILH \]
\[ P_{123}(n,m) := P_1(n,m) \cdot P_2(n,m) \cdot P_3(n,m) \]
\[ P_{45}(n,m) := P_4(n,m) \cdot P_5(n,m) \]

\[ s_{Fluct}(n,m) := 101 \cdot P_{123}(n,m) \cdot P_{45}(n,m) \cdot P_6(n,m) \cdot P_7(n,m) \cdot LH8(n,m) \cdot Ilast \]

\[ r_{Fluct}(n,m) := \begin{bmatrix} (s_{Fluct}(n,m))_{1,0} \\ (s_{Fluct}(n,m))_{0,0} \end{bmatrix}^2 \]

\[ r_{Fluct_{23,m0.5}} := r_{Fluct}(n,m) \]
\( \text{cutoff level} - R_{pbg} \)

\[
q_p(n,m) := \text{if}(r\text{Fluct}_n, m > 0.999, \lambda_m, 0)
\]

\[
q_s(n,m) := \text{if}(r\text{Fluct}_n, m > 0.999, \lambda_m, 0)
\]

\[
q_{p,p} := q_p(n,m)
\]

\[
q_{s,s} := q_s(n,m)
\]

\[
b_p(n,m) := \begin{cases} 
q_p(n,m) & \text{if } q_p(n,m) > 0 \land q_p(n,m-1) = 0 \\
q_p(n,m-1) & \text{if } q_p(n,m-1) > 0 \land q_p(n,m) = 0 \\
0 & \text{if } q_p(n,m-1) = 0 \land q_p(n,m) = 0
\end{cases}
\]

\[
b_s(n,m) := \begin{cases} 
q_s(n,m) & \text{if } q_s(n,m) > 0 \land q_s(n,m-1) = 0 \\
q_s(n,m-1) & \text{if } q_s(n,m-1) > 0 \land q_s(n,m) = 0 \\
0 & \text{if } q_s(n,m-1) = 0 \land q_s(n,m) = 0
\end{cases}
\]
\[ b_{p, m} := b_p(n, m) \quad b_{s, m} := b_s(n, m) \]

\[ q_{s, 2} = 1.01 \]

\[ b_{p, 1} = 0 \quad b_{s, 1} = 0 \]
Appendix IV

The parameters of the photonic crystal structure used in the simulations

Chapter 3 Multicomponent Photonic Crystals

Section 3.4.1 Engineering of the optical contrast: Normal incidence of light.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>10</td>
</tr>
<tr>
<td>Lattice constant, $a$ ($\mu$m)</td>
<td>3</td>
</tr>
<tr>
<td>Refractive index of Si, $n_H = n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Thickness of $t$-layer, $d_t$ ($\mu$m)</td>
<td>0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4</td>
</tr>
<tr>
<td>Refractive index of $t$-layer, $n_t$</td>
<td>1.5, 2.21</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>Normal incidence, $\theta = 0^\circ$</td>
</tr>
</tbody>
</table>
### Section 3.4.2 Oblique incidence of light: Omni-directional properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>10</td>
</tr>
<tr>
<td>Lattice constant, $a$ (µm)</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, $f_{Si}$</td>
<td>0.3, 0.3</td>
</tr>
<tr>
<td>Thickness of Si wall, $d_{Si}$ (µm)</td>
<td>0.9</td>
</tr>
<tr>
<td>Refractive index of Si, $n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Thickness of $t$-layer, $d_{t}$ (µm)</td>
<td>0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4</td>
</tr>
<tr>
<td>Refractive index of $t$-layer, $n_{t}$</td>
<td>1.5, 2.21</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>0°; 5°; 10°; 15°; 20°; 25°; 30°; 35°; 40°; 45°; 50°; 55°; 60°; 65°; 70°; 75°; 80°; 85°</td>
</tr>
</tbody>
</table>

### Section 3.5.1 Suppression of Photonic Band Gaps

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>5</td>
</tr>
<tr>
<td>Lattice constant, $a$ (µm)</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, $f_{Si}$</td>
<td>0.08...0.1</td>
</tr>
<tr>
<td>Thickness of Si wall, $d_{Si}$ (µm)</td>
<td>0.24...0.3</td>
</tr>
<tr>
<td>Refractive index of Si, $n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Thickness of $t$-layer, $d_{t}$ (µm)</td>
<td>0.3</td>
</tr>
<tr>
<td>Refractive index of $t$-layer, $n_{t}$</td>
<td>1.5</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>0°</td>
</tr>
</tbody>
</table>
### Section 3.5.2 Influence of the additional component thickness

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, ( N )</td>
<td>5</td>
</tr>
<tr>
<td>Lattice constant, ( a (\mu m) )</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, ( f_{Si} )</td>
<td>0.117</td>
</tr>
<tr>
<td>Thickness of Si wall, ( d_{Si} (\mu m) )</td>
<td>0.351</td>
</tr>
<tr>
<td>Refractive index of Si, ( n_H=n_{Si} )</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, ( n_{air} )</td>
<td>1</td>
</tr>
<tr>
<td>Thickness of t-layer, ( d_t (\mu m) )</td>
<td>0.4, 0.6, 0.8</td>
</tr>
<tr>
<td>Refractive index of t-layer, ( n_t )</td>
<td>1.5</td>
</tr>
<tr>
<td>Angle of incident light, ( \theta )</td>
<td>0°</td>
</tr>
</tbody>
</table>

### Section 3.5.3 Influence of the oblique incidence of light

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, ( N )</td>
<td>5</td>
</tr>
<tr>
<td>Lattice constant, ( a (\mu m) )</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, ( f_{Si} )</td>
<td>0.18</td>
</tr>
<tr>
<td>Thickness of Si wall, ( d_{Si} (\mu m) )</td>
<td>0.54</td>
</tr>
<tr>
<td>Refractive index of Si, ( n_H=n_{Si} )</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, ( n_{air} )</td>
<td>1</td>
</tr>
<tr>
<td>Thickness of t-layer, ( d_t (\mu m) )</td>
<td>0.6</td>
</tr>
<tr>
<td>Refractive index of t-layer, ( n_t )</td>
<td>1.5</td>
</tr>
<tr>
<td>Angle of incident light, ( \theta )</td>
<td>60°</td>
</tr>
</tbody>
</table>
### Section 3.6 Photonic Crystal ultra-wide pass-band filter

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>3</td>
</tr>
<tr>
<td>Lattice constant, $a$ ((\mu)m)</td>
<td>4</td>
</tr>
<tr>
<td>Filling fraction of Si, $f_{Si}$</td>
<td>0.25...0.33, 0.10...0.17</td>
</tr>
<tr>
<td>Refractive index of Si, $n_H=n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Thickness of $t$-layer, $d_t$ ((\mu)m)</td>
<td>0.72</td>
</tr>
<tr>
<td>Refractive index of $t$-layer, $n_t$</td>
<td>Refractive index of SiO2 in MIR from 1 to 8 (\mu)m.</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>0°</td>
</tr>
</tbody>
</table>

### Chapter 4 Microcavity Photonic Crystals

#### Section 4.2 Basic Concept: Modelling of 1D micro-cavity PhC

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>7.5</td>
</tr>
<tr>
<td>Lattice constant, $a$ ((\mu)m)</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, $f_{Si}$</td>
<td>0.243</td>
</tr>
<tr>
<td>Refractive index of Si, $n_H=n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, $n_{cav}^{1,2,3}$</td>
<td>1.5, 2.0</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>0°</td>
</tr>
</tbody>
</table>
### Section 4.3.1.1 “Si-air-Si” Fabry-Perot resonator

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, N</td>
<td>1.5</td>
</tr>
<tr>
<td>Lattice constant, ( a ) (( \mu )m)</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, ( f_{Si} )</td>
<td>0...1</td>
</tr>
<tr>
<td>Refractive index of Si, ( n_H=n_{Si} )</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, ( n_{air} )</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, ( n_{cav}^{1,2,3} )</td>
<td>1</td>
</tr>
<tr>
<td>Angle of incident light, ( \theta )</td>
<td>0°</td>
</tr>
</tbody>
</table>

### Section 4.3.1.2 “Si-LC-Si” Fabry-Perot resonator

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, N</td>
<td>1.5</td>
</tr>
<tr>
<td>Lattice constant, ( a ) (( \mu )m)</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, ( f_{Si} )</td>
<td>0...1</td>
</tr>
<tr>
<td>Refractive index of Si, ( n_H=n_{Si} )</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, ( n_{air} )</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, ( n_{cav}^{1,2,3} )</td>
<td>1.49</td>
</tr>
<tr>
<td>Angle of incident light, ( \theta )</td>
<td>0°</td>
</tr>
</tbody>
</table>
### Section 4.3.1.3 Photonic Crystal with "optical defect"

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, ( N )</td>
<td>3</td>
</tr>
<tr>
<td>Lattice constant, ( a (\mu m) )</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, ( f_{Si} )</td>
<td>0...1</td>
</tr>
<tr>
<td>Refractive index of Si, ( n_{H} = n_{Si} )</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, ( n_{air} )</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, ( n_{cav}^{1,2,3} )</td>
<td>1.49...1.69</td>
</tr>
<tr>
<td>Angle of incident light, ( \theta )</td>
<td>0°</td>
</tr>
</tbody>
</table>

### Section 4.3.2.1 Fabry-Perot resonator fabricated by anisotropic etching of (110) Si

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, ( N )</td>
<td>1.5</td>
</tr>
<tr>
<td>Lattice constant, ( a (\mu m) )</td>
<td>4.6</td>
</tr>
<tr>
<td>Thickness of Si wall, ( d_{Si} (\mu m) )</td>
<td>1.2</td>
</tr>
<tr>
<td>Thickness of cavity, ( d_{c} (\mu m) )</td>
<td>3.4</td>
</tr>
<tr>
<td>Refractive index of Si, ( n_{H} = n_{Si} )</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, ( n_{air} )</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, ( n_{cav}^{1,2,3} )</td>
<td>1</td>
</tr>
<tr>
<td>Angle of incident light, ( \theta )</td>
<td>0°</td>
</tr>
</tbody>
</table>

189
Section 4.3.2.2 Fabry-Perot resonator fabricated on (100) Si by Deep Reactive Ion Etching

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>1.5</td>
</tr>
<tr>
<td>Lattice constant, $a$ (μm)</td>
<td>8</td>
</tr>
<tr>
<td>Thickness of Si wall, $d_{Si}$ (μm)</td>
<td>2.6</td>
</tr>
<tr>
<td>Thickness of cavity, $d_{c}$ (μm)</td>
<td>5.4</td>
</tr>
<tr>
<td>Refractive index of Si, $n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, $n_{cav}^{1,2,3}$</td>
<td>1.53</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>$0^\circ$</td>
</tr>
</tbody>
</table>

Section 4.3.3.1 Thermo-tunable single channel devices

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>1.5</td>
</tr>
<tr>
<td>Lattice constant, $a$ (μm)</td>
<td>4.8</td>
</tr>
<tr>
<td>Thickness of Si wall, $d_{Si}$ (μm)</td>
<td>1.2</td>
</tr>
<tr>
<td>Thickness of cavity, $d_{c}$ (μm)</td>
<td>3.6</td>
</tr>
<tr>
<td>Refractive index of Si, $n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, $n_{cav}^{1,2,3}$</td>
<td>1.54, 1.67</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>$0^\circ$</td>
</tr>
</tbody>
</table>
### Section 4.3.3.2 Electrically tunable Fabry-Perot resonator

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>1.5</td>
</tr>
<tr>
<td>Lattice constant, $a$ (µm)</td>
<td>5</td>
</tr>
<tr>
<td>Thickness of Si wall, $d_{Si}$ (µm)</td>
<td>0.6</td>
</tr>
<tr>
<td>Thickness of cavity, $d_{c}$ (µm)</td>
<td>7.4</td>
</tr>
<tr>
<td>Refractive index of Si, $n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, $n_{cav}^{1,2,3}$</td>
<td>1, 1.45, 1.67</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>$0^\circ$</td>
</tr>
</tbody>
</table>

### Section 4.4 Coupled multi-cavity Photonic Crystal resonators

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, $N$</td>
<td>7.5</td>
</tr>
<tr>
<td>Lattice constant, $a$ (µm)</td>
<td>0.573</td>
</tr>
<tr>
<td>Thickness of Si wall, $d_{Si}$ (µm)</td>
<td>0...0.573</td>
</tr>
<tr>
<td>Thickness of cavity, $d_{c}$ (µm)</td>
<td>0.573...0</td>
</tr>
<tr>
<td>Refractive index of Si, $n_{Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, $n_{cav}^1$</td>
<td>1.74...1.52</td>
</tr>
<tr>
<td>Refractive index of cavity, $n_{cav}^2$</td>
<td>1.63</td>
</tr>
<tr>
<td>Refractive index of cavity, $n_{cav}^3$</td>
<td>1.52...1.74</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>$0^\circ$</td>
</tr>
</tbody>
</table>
### Section 4.4.5 Optimization: Compensation of the fabrication tolerances

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of periods, ( N )</td>
<td>7.5</td>
</tr>
<tr>
<td>Lattice constant, ( a ) (( \mu \text{m} ))</td>
<td>0.9</td>
</tr>
<tr>
<td>Filling fraction of Si, ( f_{\text{Si}} )</td>
<td>0.4</td>
</tr>
<tr>
<td>Refractive index of Si, ( n_H = n_{\text{Si}} )</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, ( n_{\text{air}} )</td>
<td>1</td>
</tr>
<tr>
<td>Refractive index of cavity, ( n_{cav}^1 )</td>
<td>1.63</td>
</tr>
<tr>
<td>Refractive index of cavity, ( n_{cav}^2 )</td>
<td>1.63</td>
</tr>
<tr>
<td>Refractive index of cavity, ( n_{cav}^3 )</td>
<td>1.63</td>
</tr>
<tr>
<td>Angle of incident light, ( \theta )</td>
<td>0°</td>
</tr>
</tbody>
</table>
Chapter 5 Photonic Crystals with structural deviations

Section 5.3 Modelling of thickness fluctuation

<table>
<thead>
<tr>
<th>Number of periods, $N$</th>
<th>7.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice constant, $a$ (μm)</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si, $f_{Si}$</td>
<td>0...1</td>
</tr>
<tr>
<td>Refractive index of Si, $n_{H=Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.004$a$ 0.0115$a$ 0.025$a$ 0.036$a$</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>0°</td>
</tr>
</tbody>
</table>

Section 5.5 Photonic crystals with a constant value of fluctuation of all wall thicknesses

<table>
<thead>
<tr>
<th>Number of periods, $N$</th>
<th>7.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice constant, $a$ (μm)</td>
<td>3</td>
</tr>
<tr>
<td>Filling fraction of Si</td>
<td>0.08 0.23 0.5 0.71</td>
</tr>
<tr>
<td>Refractive index of Si, $n_{H=Si}$</td>
<td>3.42</td>
</tr>
<tr>
<td>Refractive index of air, $n_{air}$</td>
<td>1</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.004$a$ 0.0115$a$ 0.025$a$ 0.036$a$</td>
</tr>
<tr>
<td>Angle of incident light, $\theta$</td>
<td>0°</td>
</tr>
</tbody>
</table>