FTIR and Raman investigation of vertically etched silicon as 1D photonic crystal

Vladimir Tolmachev^{**a}, Tatiana Perova^{*b}, Jagdish Vij^b, Ekaterina Astrova^a, Kevin Berwick^b and Alan Moore^b

^aIoffe Physico-Technical Institute, St.-Petersburg, Russia; ^bDept. Electr. & Electr. Eng., Trinity College, Ireland; ^cDept. of Electr. & Communic. Eng., DIT, Ireland

ABSTRACT

The reflection spectra of composite materials on a base of grooved silicon and grooved silicon infiltrated with nematic liquid crystal (LC) have been calculated using the optimal parameters of a grooved silicon matrix suitable for the infrared range. The grooved silicon structures with different lattice constants ($A=16, 12, 8$ and $4 \mu\text{m}$) have been designed and prepared. An important parameter of these structures is the thickness of the silicon walls (D_{Si}). This has been obtained using simulations of the spectra. This parameter was used for further analysis of the spectra of composite material “grooved Si-LC”. The experimental reflection reaches a maximum of 65% (with signal modulation from maximum to minimum up to 55%) for the composite structures with a small number of lattice periods. This makes these structures very attractive for a number of potential applications. The analysis of the polarised infrared spectra of Si structures infiltrated with LC allows one to determine the orientation and the refractive index (N_{LC}) of the liquid crystal. For the samples with a distance between Si walls of $6\text{--}10 \mu\text{m}$, it was found that the refractive index was $N_{\text{LC}} \approx 1.5$ for p-polarised light and $N_{\text{LC}} \neq 1.5$ for s-polarised light. This leads to the conclusion on the planar orientation of liquid crystal molecules with respect to the Si walls. For the samples with a distance between Si walls less than $3 \mu\text{m}$, a homeotropic alignment of liquid crystal molecules has been found. Micro-Raman spectroscopy has been applied for analysis of stress in such Si structures. The maximum stress of about 2 GPa was obtained on the top of Si walls (under the silicon dioxide layer).

Keywords: Photonic crystals; silicon; Fourier transform infrared spectroscopy; micro-Raman spectroscopy

1. INTRODUCTION

Photonic crystals (PC) are materials with a regular change in the refractive index, N , with periodicity of the order of the wavelength [1]. PC may have periodicity in one (1D), two or three dimensions. Among the most familiar examples of 1D photonic crystals are the interference coatings on gold. At the right choice of N and the optical thickness of the layers $N \cdot D$ (where D is the geometrical thickness of the layer with corresponding value of N) for the certain range of wavelength λ , the band with maximum reflectance (up to 100%) will appear in the reflection spectra R . This band is called a photonic band gap (PBG) since it possesses a forbidden gap for photons of certain frequency range, similar to that for electrons in atomic crystals. There are a few different technological methods for preparation of 1D periodical structures. One method is the electrochemical etching of silicon in a HF solution with formation of nano-porous periodical structures with different porosities [2,3]. For such structures, the ratio of the refractive indices of the different layers (so called optical contrast) plays an important role. As larger the ratio, the wider is the total reflection band and the lower are the number of layers that can be formed. From this point of view, the choice of the pair “Si-air” is very promising, since such a medium possesses an extremely high contrast ratio (3.42/1 in the IR range). Structures with a great number of Si walls separated by air intervals (so called grooved Si) can be obtained by vertical anisotropic etching of $\langle 110 \rangle$ Si in an alkaline solution through an oxide mask [4]. Fig. 1 shows the SEM image of a grooved Si structure obtained by this method. To our best knowledge, the optical properties (reflection and transmission spectra) of this composite material in the middle infrared range were never studied before, despite the fact that Kendall [4] suggested their use as optical filters for the far-infrared region.

[*perovat@tcd.ie](mailto:perovat@tcd.ie); phone 353 1 608-3802; fax 353 1 677-2442; <http://www.tcd.ie>; Department of Electronic & Electrical Engineering, University of Dublin, Trinity College, Dublin 2, Ireland; **tva@mail.ioffe.ru; phone 7 812 247 9957; Ioffe Physico-Technical Institute, Polytechnicheskaya Str.. 26, St.-Petersburg, Russia.

Furthermore, the position and the width of PBG can be tuned over a wide spectral range - the tuning being provided by varying the crystal lattice parameters and dielectric constants of materials composing PC. The possibility to tune the PBG structure in real time is a challenging task. It can be achieved by utilisation of substances with the ability to change their refractive index under external forces. The general concept of tunable PBG in PC filled with liquid crystals has recently been formulated [5]. Tunable PCs were obtained by impregnation of LC in artificial opal [6] and macro-porous Si matrices [7]. The PBG position in these composites depends on temperature due to LC phase transition. The most interesting task is to tune the PBG with an electric field. First attempts to obtain the electro-optical effect in opal based composite PC [8] revealed a lot of problems and demonstrated that we are still in the early stages towards practical applications of tunable PCs.

Recently, investigations into the infiltration of the commercially available LC mixture SCE-8 and triphenylene based discotic LC into macroporous Si matrices have been carried out [9]. A new IR method for determining the LC alignment in the mesophase has been proposed. Using this method, the alignments of two types of LCs infiltrated into a macroporous Si matrix have been determined.

The high contrast ratio of grooved Si in the IR range, the presence of the smooth vertical walls and the possibility of the wide variety in the design and technology of such structures, allow us to suggest it as a matrix for the preparation of a new composite material "grooved Si-LC". The advantage of this structure also lies in its simplicity which aids theoretical simulations and thus simplifies the interpretation of experimental results. Therefore, the main objective of this study was i) investigation of the possibility to infiltrate grooved Si structures with LC, ii) measurement and analysis of IR spectra obtained from composite materials, and iii) investigation of strain in these structures using micro-Raman spectroscopy.

2.EXPERIMENTAL

2.1 Sample preparation

The best geometrical parameters of periodical Si structures based on theoretical simulations were estimated before the structure preparation. The optimal width of Si walls (D_{Si}) as well as air intervals (D_{air}) as shown in Fig. 1 can be chosen from the following ratio $D \sim \lambda_0 / (N \cdot 4)$, where λ_0 is the wavelength with respect to which the calculation of the high-reflected structure has been made. The deep ($> 100 \mu m$) and very narrow grooves have already been fabricated (see Ref. [5]) but no investigations were carried out on how to obtain very narrow Si walls. The problem of mechanical durability arises with the decreasing width of the Si walls. As a result of this, there appears to be an additional problem with the design of these structures to make them more stable. In order for the Si walls to be more durable after the etching process, the construction contained additional Si support squares to which the grooved Si structure is attached (see Fig. 2). These Si squares also permit easier handling of the samples during measurements. Using the procedure described elsewhere [10], four grooved Si samples were created: three with lattice constant $A=16, 8$ and $4 \mu m$ - each wafer with number of Si walls $m=50$ and one sample with $A=12 \mu m$ and $m=3$. The lattice constant A may be written as: $A=D_{Si} + D_{air}$.

The Si structures were infiltrated by commercial nematic liquid crystal E7 in a manner described in Ref. [9]. Controlled filling of the grooves with LC has been achieved using optical microscopy (see Fig. 6).

2.2 Method of FTIR measurements

FTIR measurements in reflection mode in the range of $700-7000 \text{ cm}^{-1}$ have been performed with a wavelength resolution of $d\lambda=0.001-0.05 \mu m$ using a Digilab FTS 6000 spectrometer in conjunction with a UMA 500 infrared microscope. IR measurements of grooved Si are 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 has been designed for the measurements (see [11] for details). This allows adjustment of the sample in X-Y-Z directions with high precision. The trajectory of the IR beam through the sample was chosen and fixed by using an optical microscope. This minimises the presence of possible defects in the Si structure through which the IR beam

will travel. Then the sample was rotated by 90° and a rectangular shaped area was chosen (see Fig. 2) for IR measurements.

Fig 1: SEM image of sample with lattice parameters $A=8 \mu\text{m}$.

Fig.2: Schematic of FTIR reflection measurements on the periodical structure of grooved Si.

Certain difficulties arose during these measurements due to the 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 [11]. The single beam reflection signal from the gold-coated glass has been used as a background. The measurements were performed in the following way: first, the reflection spectrum in single beam mode was collected from the sample aligned with a great care and then the microscope transportation stage was moved to the gold-coated glass, which was placed beside the sample at the same level. All FTIR measurements were made with a polariser placed before the microscope detector with the electric vector of p -polarised light directed along the Si walls (see Fig. 2).

3. ANALYSIS OF THE REFLECTION SPECTRA

The analysis of the reflection spectra involves:

- 1) obtaining the calculated spectra, based on the estimated parameters of the periodical structure, D_{Si} ,
- 2) variation of this parameter and comparison of the calculated spectra with the experimental ones,
- 3) estimating the fitting quality and determining the most satisfactory parameter of D_{Si} .

3.1 Calculation of the optical parameters of the periodical structures

In this work, an approach considering the propagation of a plane wave through the periodical structure by taking into account the multiple reflections taking place at each interface has been used. All the calculations have been performed using the method of characteristic matrix [12], considering the matrix of the multilayer film:

$$S = I_{i-1} \cdot L_i \cdot I_i \cdot L_{i+1} \cdot \dots \cdot I_{m-1} \cdot L_m \cdot I_{m+1} \quad (1)$$

where I is the matrix of the reflection for the respective interface border (2) and L is the matrix of the transmission for each layer (5):

$$I_i = \begin{pmatrix} 1 & r_i \\ r_i & 1 \end{pmatrix} \quad (2)$$

$$r_i = \frac{N_i - N_{i-1}}{N_i + N_{i-1}} \quad (3)$$

$$t_i = \frac{2 N_{i-1}}{N_i + N_{i-1}} \quad (4)$$

$$L_i = \begin{bmatrix} e^{j\beta_i} & 0 \\ 0 & e^{-j\beta_i} \end{bmatrix} \quad (5)$$

$$\beta_i = 2\pi \left(\frac{D}{\lambda} \right) N_i \quad (6)$$

λ is the wavelength, N is the refractive index and D is the thickness of the layer

Since the alternating layers have the same value of the consequent matrix, equation (1) was transformed to a more convenient equation (7) that can be programmed

$$S = [(I \cdot L)_A \cdot (I \cdot L)_B]^m \cdot (I \cdot L)_A \quad (7)$$

where $(I \cdot L)_A$ and $(I \cdot L)_B$ are the matrix products at the border of the high-refractive (A) and low-refractive (B) layers respectively, m is the number of structure periods.

The reflection coefficient, $R(\lambda)$, has been calculated using the following expression:

$$R(\lambda) = | [S(\lambda)_{1,0} / S(\lambda)_{0,0}]^2 | \quad (8)$$

For calculations the following parameters for N and k are used: for the high-refraction layer, $N_{Si}=3.42$ and $k_{Si}=0$; for low-refraction layer $N_{air}=1$. The Si wall width, D_{Si} , and air interval, D_{air} , were used as variable parameters.

The experimental reflection spectra in p -polarisation for the structure with the lattice constant $A=8 \mu m$ is shown in Fig. 3. It should be noted that since for the empty grooved structures the spectra measured in s - and p - polarisations are the same, the spectrum for only one polarisation will be shown. The best spectrum obtained from the fitting procedure with parameters $D_{Si}=1.8 \mu m$ and $D_{air}=6.2 \mu m$ is shown in Fig. 3 for comparison. The fitting accuracy is usually obtained around $D_{Si} = \pm 0.1 \mu m$. Good agreement between experimental and calculated maxima and minima of spectra can be seen in Fig. 3. The ratio between the optical paths of the high-refractive and low-refractive structures was found to be equal to $(N \cdot D)_{Si} / (N \cdot D)_{air} = (1.8 \cdot 3.42)_{Si} / (1 \cdot 6.2)_{air} = 6.15/6.2 \approx 1$. Such a spectrum is close to the ideal $\lambda/4$ calculated with the lattice constant $A = 8 \mu m$. The calculated PBG range is located in the far-infrared range ($\lambda = 18-39 \mu m$) and is not available in our experimental set-up. However, the secondary band gap with a reasonable spectral width ($\sim 1 \mu m$) and sharp slope can be seen in the region of $\lambda = 8-9 \mu m$.

A similar analysis was performed for the sample with the smaller lattice constant ($4 \mu m$) and PBG in the range of $\lambda \sim 10-20 \mu m$ (Fig. 4) was anticipated. This spectrum is more noisy compared with the previous experimental data shown in Fig. 3. This is because the groove's depth was only $30 \mu m$ for the second sample, which required the decreased aperture of the IR beam. The best fitting was obtained for the structure parameters of $D_{Si}=1.2$ and $D_{air}=2.8 \mu m$ and show good agreement with the main maxima and minima (see Fig. 4). In accordance with calculations performed with these parameters, the main PBG lies in the range $\lambda=10-22 \mu m$ and can be partly identified (up to $\lambda=14 \mu m$) experimentally.

Based on the analysis of the obtained data, it should be noted that the agreement between the experimental and theoretical maxima and minima for most structures presented here confirms the appropriateness of the chosen model and the high quality of the interfaces. The position of the secondary maxima is more sensitive to deviation from the nominal parameters for the structure. This allows the use of these particular maxima for fitting control purposes. The good agreement between experimental and theoretical spectra in the mid-infrared range suggests that there is a high probability of the existence of the main PBG for 1D photonic crystals in the far-infrared (FIR) region. Measurements in this region were not carried out for this work. We suggest that the secondary stop bands can also serve as a photonic band gaps due to their high contrast, width ($\geq 1-2 \mu m$) and sharpness of their edges.

The parameters of the grooved Si matrix necessary for fitting experiment with theory are listed in Table 1. For the purposes of these calculations, it was assumed that the refractive index of the LC must be ~ 1.6 after the

impregnation of LC into the Si grooves. This value of the refractive index is an average between ordinary ($N_o=1.5$) and extraordinary ($N_e=1.7$) refractive indices existing in the anisotropic state of this LC. The above mentioned parameters are given in Table 1 for different lattice constants $A=16, 12, 8$ and $4\ \mu\text{m}$. The real parameters, D_{si} and D_{air} , obtained during the fitting procedure and calculated regions of PBG_{air} are also listed in Table 1. The latter was calculated for the empty grooves.

Fig3. Calculated (1) and experimental (2) reflection spectra of sample N5 with lattice parameter $A=8\ \mu\text{m}$.

Fig.4 : Calculated (1) and experimental (2) reflection spectra of sample N7 with lattice parameter $A=4\ \mu\text{m}$.

We found, from the comparison of data for all three samples prepared with the lattice constant $A=16\ \mu\text{m}$, the experimental parameters D_{si} do not coincide with the calculated ones. The reason for this could be as follows: during the sample preparation, etching occurs not only in the vertical direction but also in the horizontal direction (over-etching or undercutting). This complicated process depends on different technological factors. As a result of the deviation of the real parameters (D_{si} and D_{air}) from the calculated ones (Table 1), we observed a certain shift of PBG_{air} in our spectra. It should be noted that these deviations influence the secondary stop bands more substantially. The latter can appear, disappear, or can be shifted or corrupted depending on the particular values of D_{si} and D_{air} . Moreover, in the case of underetching, technologically there is a possibility to etch the Si walls up to estimated value of D_{si} . For example, samples N2 and N3 still can be etched up to the required thickness, while sample N1 was already overetched to thickness D_{si} .

Samples N5 and N6 ($A=8\ \mu\text{m}$ and $D_{\text{si}}=1.8$ and $2.0\ \mu\text{m}$) are not suitable for application as a medium for the composite grooved Si-LC preparation due to over-etching (seen as a deviation from the calculated value of $D_{\text{si}}=2.55\ \mu\text{m}$). At the same time, sample N5 shows quite reasonable parameters ($D_{\text{si}}=1.81\ \mu\text{m}$) for using it as a photonic crystal without infiltration. Due to this, the reflection spectrum of this sample consists only of characteristic secondary bands ($\lambda=8-9, 5\ \mu\text{m}$ etc.) i.e. it is an optimal sample. Sample N6 is also overetched despite its PBG_{air} being shifted to the short wavenumber range of spectra ($\lambda=8.5\ \mu\text{m}$). Sample N7 has parameters very close to those calculated ($D_{\text{si}}=1.2\ \mu\text{m}$) and therefore the spectrum (see Fig. 4) is close to the spectrum of a photonic crystal with optimal parameters.

Thus, we can find that the reflection spectra of grooved Si samples with different lattice constants were investigated and the parameters of their periodical structures (D_{si} and D_{air}) determined. The latter will be used for the analysis of the composites grooved Si-LC.

4. MICRO-RAMAN MEASUREMENTS AND ANALYSIS

Raman spectra were registered in backscattering geometry using a RENISHAW 1000 micro-Raman system equipped with a Leica microscope. The excitation wavelength was 514.5 nm from an Ar⁺ ion laser (Laser Physics Reliant 150 Select Multi-Line) with a typical laser power of ~ 20 mW. An 1800 lines/mm grating was used in all measurements, which corresponds to a spectral resolution of ~ 2.5 cm⁻¹. The 100x magnifying objective of the Leica microscope focused the beam into a spot of about 0.7 μm in diameter. In order to define the position of the phonon lines with a higher accuracy, the spectral lines, used for the analysis, were fitted with a Lorentzian function. The removal of the background baseline followed by a line fit using a Lorentzian function allows three components of the Raman spectrum to be determined viz. intensity, half width and position. These variations are related to the composition, defect density, and magnitude of stress respectively. The position of this band, as was shown in the early eighties, is very sensitive to stress in silicon. The shift of this band ($\Delta\omega$) under stress from its position for the stress free silicon lattice (ω_{ref}) allows one to define the magnitude of stress (σ) using a simple equation for the case of the uniaxial stress:

$$\Delta\omega = -2 \times 10^{-9} \sigma \text{ . (Pa)} \quad (9)$$

Here, $\Delta\omega = (\omega_{stress} - \omega_{ref})$ (in cm⁻¹) and ω_{stress} is the peak frequency of the phonon band of silicon under the stress. A positive or negative shift in the Raman peak position corresponds to compressive or tensile stress, respectively, assuming uniaxial stress only i.e. within the plane of the wafer.

The schematic of Raman measurements for these samples is shown in Fig. 5. Raman measurements performed from the side of the grooves show quite large stress on the top of Si walls (under the SiO₂ layer), which is varied from 1 to 2 Gpa for different samples. This stress was decreased substantially after the oxide removal. The Raman line-mapping experiment shows also the decrease of stress when measurements are performed from the top to the bottom of Si walls (as shown in Fig. 5).

Table 1.

The optical parameters of grooved Si matrix for composite photonic crystals.

Calculated parameters for the composite system, μm		The parameters obtained from IR spectra, μm			Sample
D_{Si}	D_{air}	D_{Si}	D_{air}	$\text{PBG}_{\text{air}}(\lambda)$	
A= 16 μm (m=50)					
5.1	10.9	4.8	11.2	41-86	N1
		5.7	10.3	45-90	N2
		6.2	9.8	49-94	N3
A= 12 μm (m=3)					
3.825	8.175	2.1	9.9	29-55	N4
A= 8 μm (m=50)					
2.55	5.45	1.8	6.2	18-39	N5
		2.0	6.0	19-42	N6
A= 4 μm (m=50)					
1.275	2.725	0.8	3.2	*8.5-19	N7
		1.2	2.8	*10.3-22	N8

*experimental measurements

m- the number of periods

Fig. 5. Schematic of stress measurements from the side (I) and from the plane (II) of Si walls of grooved sample using Raman scattering.

Fig. 6. Top view of sample N4 ($m=4$) with lattice parameter $A=12\ \mu\text{m}$ after impregnation with liquid crystal (LC).

5. ANALYSIS OF THE REFLECTION SPECTRA OF SAMPLES IMPREGNATED WITH LIQUID CRYSTAL

The analysis of spectra consists of:

- 1) comparison of spectra of grooved Si samples, both empty and impregnated with LC
- 2) obtaining the calculated spectra, using the parameters of matrixes (periodical structure) D_{Si} and assumed parameter of the refractive index N_{LC} of LC
- 3) the variation of the parameter N_{LC} and comparison of the calculated and experimental spectra.
- 4) determination of the more suitable parameters, N_{LC} , for sample under investigation at certain polarisations of the IR beam.

The calculated spectra were obtained in the same way as previously described. The experimental spectra were measured with p - and s -polarised IR light. The rod-like molecules of nematic LCs can be oriented parallel and perpendicular to the Si walls. For the nematic LC used in this study $N_o=1.5$ and $N_e=1.67$ [12]. LC contained in grooved Si can influence the reflection and transmission spectra of the composite. Under the influence of external forces (temperature or electric fields), the orientation of LC molecules may change which, in turn, will change N and finally change the reflection (transmission) spectrum of the system.

Fig. 7 shows the reflection spectra of grooved Si matrix before and after the filling of grooves with LC. From this figure, the shift of the bands, their distortion and an appearance of the new reflection bands can clearly be seen. This is due to the change in refractive index of the grooves from $N=1$ (for empty grooves) up to 1.5-1.7 (filled with LC). We found that fitting of the reflection spectra from samples impregnated with LC was more difficult than for the empty ones. Possibly this is connected with the peculiarity of the optical properties of LC filled in grooves.

It is well known that the simple alignment of liquid crystals (nematic LC in particular) can be done by slow cooling from the isotropic phase to the mesophase. In our experiment, heating the samples to the temperature of the isotropic phase of LC ($\sim 70^\circ\text{C}$) followed by slow cooling to room temperature did not affect the reflection spectra for almost all samples. This implies that the orientation of LC in grooves is nearly the same as after the sample filled the grooves with LC in mesophase (at room temperature). Thus the reflection spectra for some samples do not demonstrate an anisotropy, while for other samples the anisotropy shown in the spectra is quite substantial (see Fig. 8). For samples impregnated with LC with a small number of periods (Figs. 5 and 6), the maximum values of R reach 65 % and the

contrast R (ΔR) reaches 55%. These parameters are very attractive for future applications of such systems in optical schemes.

Fig.7: The experimental reflection spectra of empty (1) and impregnated with LC (2) samples with lattice parameter $A=16 \mu\text{m}$.

Fig.8: The experimental reflection spectra of sample impregnated with LC with the lattice parameters $A=12 \mu\text{m}$ for p - and s -polarisations.

Then we performed the fitting of the refractive index N_{LC} of LC filled in a grooves. This was done through a comparison of the experimental and calculated spectra for p - and s -polarised light, where N_{LC} was taken as a fitting parameter. The same model which was described above (section 3.1) is used here. Typically, the accuracy achieved was approximately $dN_{LC} = \pm 0.1 \mu\text{m}$ (if $dN_{LC} > 0.01$, then see the range of N_{LC} shown in Table 2).

Table 2.

The optical parameters of composite photonic crystals based on grooved Si and nematic liquid crystal E7.

Parameters of matrix and PBG,μm			N _{LC}				Sample
			Before heating		After the heating		
D _{si}	D _{LC}	PBG _{LC} (λ)	N _{LC} (p)	N _{LC} (s)	N _{LC} (p)	N _{LC} (s)	
* A= 16 μm (m=50)							
5.7	10.3	55-94 _{1.5} 60-95 _{1.7}	-	-	1.5	1.6	N2LC
6.2	9.8	57-96 _{1.5} 62-97 _{1.7}	1.5	1.69	1.5	1.67	N3LC
A= 8 μm (m=50)							
2.5	5.5	27-45 _{1.5} 30-47 _{1.7}	1.5	1.55-1.65	1.5	1.55-1.65	N9LC
A= 4 μm (m=50)							
0.8	3.2	12.4-20 _{1.5} 13.9-20.5 _{1.7}	1.5	1.5	1.5	1.5	N7LC
1.2	2.8	13.2-22.4 _{1.5} 14.6-22.7 _{1.7}	1.57	1.57	1.53	1.54	N8LC

*The subscript in this column shows the N_{LC} value used at calculations of PBG

As can be seen from Table 2, if the values of $N_{LC}=1.5$ and 1.7 (see subscripts in column PBG) were used during the calculation then we can expect the shift of short wavenumber edge of PBG for $A=16 \mu\text{m}$ structure on $d\lambda=5 \mu\text{m}$, for

$A=8\text{ }\mu\text{m}$ on $d\lambda=3\text{ }\mu\text{m}$ and for $A=4\text{ }\mu\text{m}$ on $d\lambda=1.5\text{ }\mu\text{m}$. The values of N_{LC} calculated from the spectra for different polarisations are equal to 1.5 for p-polarisation and ranging from 1.5 to 1.65 for s-polarisation. The calculations performed for spectra at s-polarisation often do not fit well. This is possibly due to the imperfections in the initial matrix (grooved Si) or due to peculiarities of the optical properties of LC when impregnated. We can see also from Table 2 that heating to the isotropic phase followed by slow cooling to room temperature does not affect the value of N_{LC} . This leads to the conclusion that the isotropic orientation is not altered by heating during filling of the grooves with LC at the mesophase temperature.

The data obtained for N_{LC} (Table 2) can serve as criteria for the orientation of LC in the grooves of the Si matrix. For example, if the values of $N_{LC}=1.5$ obtained for p-polarisation are not the same as for s-polarisation, then it suggests a planar orientation of LC molecules with respect to the Si walls for samples with air spaces ranging from $6\text{ }\mu\text{m}$ to $10\text{ }\mu\text{m}$ (samples N2LC, N3LC and N9LC). For sample NLC7, the value of $N_{LC}=1.5$ was obtained for both (s- and p-) polarisations. This is possible only if the orientation of LC in grooved matrix is homeotropic with respect to the Si walls. D_{LC} for this particular sample is only $3\text{ }\mu\text{m}$ and possibly the decrease of the space between the Si walls is the reason for this type of orientation. The influence of the properties of a grooved Si matrix on LC alignment will be investigated in detail in the near future.

6. CONCLUSION

The reflection spectra of composite photonic crystal on the basis of Si and liquid crystal have been calculated based on the optimal parameters of the matrix of the periodical structure (grooved Si) for the IR region. Grooved Si structures with different lattice constants (16 , 12 , 8 and $4\text{ }\mu\text{m}$) were designed and prepared. FTIR reflection method for measurements of grooved Si systems is developed. The analysis of the spectral characteristics of the matrix has been performed theoretically, which shows high sensitivity of the secondary band gaps to the deviation from the optimal parameters during the fitting procedure. This can be used for the spectral simulation. Theoretical analysis of the reflection spectra allows one to define the parameters of the periodic structure (thickness of Si walls) which was used at a later stage during the analysis of the composite system - grooved Si and liquid crystal.

For the empty sample with lattice constant $A=4\mu\text{m}$, the main photonic band gap was found in the region $10\text{--}22\text{ }\mu\text{m}$, which was confirmed experimentally up to $14\text{ }\mu\text{m}$. It was shown that the spectra of some composite materials "grooved Si-LC" do not possess a strong anisotropy while the spectra of others show quite strong anisotropy of the optical properties. The analysis of the polarised spectra of grooved Si impregnated with LC allows one to determine the refractive index of LC and the orientation of its molecules. It was found that if $N_{LC}=1.5$ for p-polarisation and $N_{LC}\neq 1.5$ for s-polarisation, then a planar orientation of the LC's molecules with respect to the Si walls (with intervals between them ranging from 6 to $10\text{ }\mu\text{m}$) is indicated. The decrease of the interval between the Si walls is probably the reason behind the homeotropic orientation of the LC's molecules.

The surface of the Si walls (from the plane and from the side) was measured with a micro-Raman spectrometer in backscattering geometry. Quite substantial stress was observed in the Si walls if the oxide mask is not etched.

For the grooved Si impregnated with nematic liquid crystal, the maximum reflection reached is 65% and the maximum contrast $R(\Delta R)$ is about 55%, which makes these composite materials very attractive for future applications.

ACKNOWLEDGMENTS

The authors wish to thank L. Granitsyna for help with sample preparation, A. Naschekin for SEM measurements and E. Vlasova for the assistance in the optical measurements. Thanks to Enterprise Ireland and to European Community for the financial support of this work through International Collaboration Programme IC/2002/069 and IC/2002/029 and INTAS 01-0642.

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