

Tunable Microcavity Based on Macroporous Silicon: Feasibility of Fabrication

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Abstract—Simultaneous electrochemical etching of deep pores and trenches in silicon was used to fabricate a two-dimensional, photonic crystal slab (PCS). The structure consists of five rows of macro-pores on both sides of a trench-defect, filled with a nematic liquid crystal. Polarized reflection and transmission spectra from the fabricated structure were investigated in the mid- infrared spectral range and were compared with spectra calculated using a scattering matrix method. In order to obtain agreement between the experimental and calculated spectra, a model structure with a complex refractive index of silicon was introduced. This enabled us to take into account losses related to light scattering at the inner surfaces of pores and trenches within the structure. The influence of these losses on the amplitude of the defects and surface Tamm states was analysed using this model. The Tamm states originate from the unstructured Si layer at the interface of the structure and the external medium, air in this case. A quantitative evaluation of the losses was performed by extracting a coefficient from a fit to the experimental spectra. This coefficient was utilised to determine the dependence of the micro-cavity parameters on the number of periods in the PCS. We conclude that a micro-cavity based on macro-porous silicon should not have more than three periods on each side of a defect.

Index Terms—Two-dimensional photonic crystals, Photonic crystal cavity, cavity mode, surface Tamm states, scattering matrix method, FTIR spectra

I. INTRODUCTION

PHOTONIC resonators, which have the capacity of light localisation, are utilized in many areas of fundamental research and technology. These structures are of a great importance for studying the processes of coherent electron-phonon interactions as well as development of ultra-small filters, low-threshold lasers, the elements of non-linear optics, quantum information systems and sensors. Silicon micro-photonics refers to photonic integrated circuits where information processing is achieved by in-plane light propagation [1]. Some of micro-photonic devices [2] require tuning of the resonance frequency in a real time.

Tuning of the spectral position of a Photonic Stop-Band (PSB) by variation of the refractive index of a Liquid Crystal (LC), infiltrated into the voids of the dielectric matrix of a Photonic Crystal (PC), was initially suggested in theoretical work described in Ref. [3]. In order to realise this idea practically, various Silicon-Liquid Crystal composite structures were investigated. One-dimensional (1D) PCs consist of trenches in single crystalline silicon, while two-dimensional (2D) PCs consist of macro-pores in silicon. Effective tuning of the band gap edges and defect states within PSBs have been achieved using electro- and thermo-optical effects in the LC filler [4], [5], [6], [7], [8]. The key issue in obtaining

a sufficiently large effect is the initial alignment of the LC director in the structure voids. The highest and reproducible shift of the PBG spectral position can be achieved when the initial homogeneous planar alignment is changed to the homeotropic one, for example, under application of an external voltage [7]. As silicon is a good electrical conductor, there is a problem in designing of electro-tunable devices based on 2D and 3D PCs. This problem can be overcome by the proposed here structure of a silicon microresonator, formed from the trench, which simultaneously divide a 2D PC into two electrically isolated parts and thus allowed to vary a refractive index of LC infiltrated into cavity under applied electric field.

In order to fabricate a 2D PC with a small number of periods, simultaneous etching of macropores and trenches in Si was suggested in Ref. [9]. Specific features of this technology were investigated in our previous papers, based on structures with a lattice period of $8\mu\text{m}$ [10], [11], [12], [13]. These structures were also used to develop the process of registering reflection and transmission spectra using a Fourier Transform Infrared (FTIR) spectrometer, combined with an IR microscope. A method to theoretically calculate the optical characteristics of these structures using the scattering matrix method, taking into account losses on the inner surfaces of the structures was also developed (see, for example [14]). These approaches were used for the fabrication and characterization of micro-cavities with various defects, located at the centre of a PC structure and infiltrated with a nematic LC [11], [13]. A characteristic feature of the PC structures fabricated is an unmodulated silicon layer at the Si-air interface. This layer may lead to the appearance of local surface states within a PSB [15].

In this study, we fabricated a composite micro-cavity structure with a lattice period $a = 3.75\mu\text{m}$ and a trench-defect, infiltrated with an LC. This structure possesses a lower PSB in the mid-IR range, and can be used for tuning the resonance peak using an external electric field. The optical properties of the structure are investigated, both experimentally and theoretically. The spectral features observed are identified, and we discuss the feasibility of fabricating the microcavity by photo-electrochemical etching.

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II. SAMPLE FABRICATION

In order to fabricate the micro-cavity (or microresonator) structure, we used n-type (100) Si wafers of resistivity $\rho = 5\Omega\cdot\text{cm}$. Two types of nucleation centers were defined on the

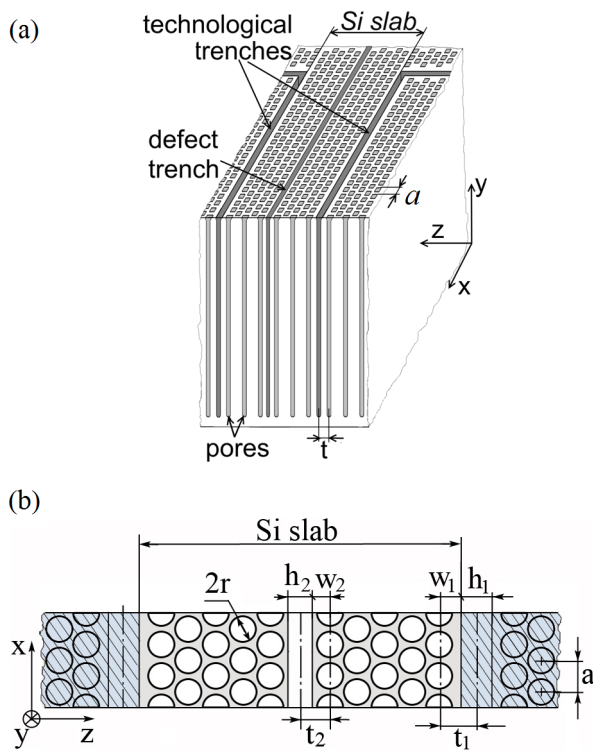


Fig. 1. Schematic of part of the sample after anodization: a) 3D picture, b) top view of a narrow fragment of the structure (the dashed regions show the removed parts of the structure).

wafer surface using photolithography. These nucleation centers were initially pits, which grew to cylindrical pores, then grooves, ultimately forming trenches during sample anodization. The anodization process was performed in a 4% aqueous solution of HF while illuminating the back side of the wafer [16]. The anodization was carried in regime which provides a constant pore diameter with depth [17]. Temperature of anodization was of 20°C. The initial current density was $j = 13 \text{ mA/cm}^2$. A detailed description of the fabrication technology can be found in Refs. [10], [13]. The substrate was detached from the structure by grinding and polishing the back of the sample. In order to increase the pore radius, the structures were subjected to an additional thermal oxidation in a wet-steam atmosphere at a temperature of 1100°C, followed by dissolution of the oxide in HF solution.

The trenches play a dual role. Firstly, the technological trenches create a closed loop, defining the active part of the structure. In addition, the trenches allow the removal of porous material from both sides of the PC slab. The trench passing through the centre of the structure forms a defect mode in the PSB. For simplicity, it will be referred to as a trench-defect in the rest of this discussion. This trench also divides the structure into two parts, isolated from each other, allowing the application of a voltage in order to create a uniform electric field in the region of the trench-defect [14]. After mechanical removal of the substrate, the sacrificial parts of the structure, surrounded by the close loop of the technological trenches, were detached from the sample. The remaining bar, oriented along the $\Gamma - K$ direction in the triangular lattice of the 2D

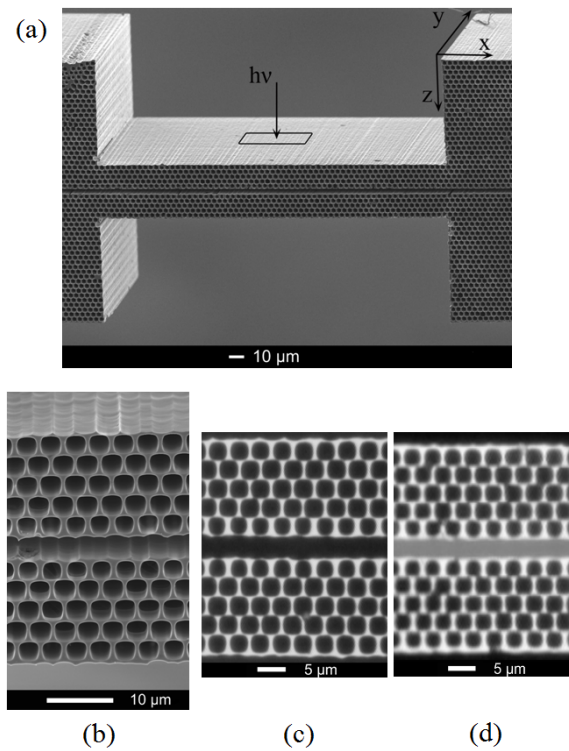


Fig. 2. Scanning Electron Microscopy (SEM) image of the micro-cavity structure a) 3D view and b) enlarged view of the central region. Optical microscopy image of the central part: c) before and d) after infiltration with the LC.

PC (X axis), formed a PCS of $\sim 38 \mu\text{m}$ width along the Z axis and of $\sim 250 \mu\text{m}$ height along the Y axis. The resonator was formed by a trench-defect, surrounded by Bragg mirrors consisting of five macropore rows on both sides (see Fig. 1a).

The geometrical parameters of the fabricated micro-cavity structure are shown in Fig. 1b. Three parameters are defined by the photomask: *viz.* the lattice period $a = 3.75 \mu\text{m}$, and the distances from the centre of the trench to the centre of the nearest row of pores, $t_1 = 4.25 \mu\text{m}$ and $t_2 = 3.55 \mu\text{m}$, for technological and defect trenches, respectively. The pore radius r is variable and depends on the anodization regime and any post anodization treatment. The width of the trenches varies in accordance with the radius of the pores. The relationship between these parameters can be expressed as $h_{1,2} = 2rm_{1,2}$. The correction factor m depends on $t_{1,2}$. This is due to the redistribution of the local current density during anodization in the regions with a different distance from the trench to the regular porous part of the structure. In our case, these parameters were determined experimentally by measuring the pore diameter and trench width in the fabricated structure. This procedure resulted in values of $m_1 = 1.04$ and $m_2 = 0.92$. As can be seen from Fig. 1b, the distances w_1 and w_2 from the edge of the trench to the centre of the pores are: $w_{1,2} = t_{1,2} - h_{1,2}/2 \equiv t_{1,2} - rm_{1,2}$.

The final structure without the LC filler is shown in Figs. 2a,b. Infiltration of the trench-defect was carried out from the face-side of the structure. The LC was held in place by capillary forces. The infiltration process was controlled by the observing the image from the back-side of the structure. The

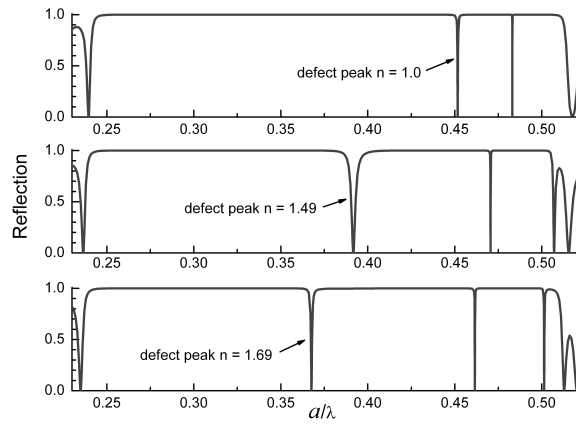


Fig. 3. Calculated reflection spectra of the micro-cavity with a trench-defect, infiltrated with fillers of different refractive indices n , shown by the numbers near the resonance peak. The filling factor $r = 0.433a$, normal incidence of light, refractive index of silicon $n_{Si} = 3.42$.

central part of the final structure before and after infiltration with the LC is shown in Figs. 2a,b. The nematic LC E7 (*Merk K GaA, Germany*) has been selected for infiltration because of its significant birefringence in the IR spectral range, $\Delta n = 0.2$ [18]. It also exhibits a room temperature mesophase. Our preliminary calculations show that the variation of refractive index of the LC from 1.49 to 1.69 under the influence of an applied electric field leads to a shift of the resonance peak by $\sim 6\%$ (see Fig. 3). Note that the lower quality factor of the resonator state for $n = 1.49$ is a result of a weak interaction between the defect and the surface mode. The surface Tamm peak at $a/\lambda = 0.4$ itself has a very low amplitude for $k = 0$ and is not observed on the spectra.

III. OPTICAL MEASUREMENTS AND CALCULATION METHOD

The reflection, R , and transmission, T , spectra of the micro-cavity were registered with a Digilab FTS 6000 FTIR spectrometer in conjunction with a UMA 500 infrared microscope in the wavenumber range from 650 to 6500 cm^{-1} . The IR light, polarized along (TM) or perpendicular (TE) to the pore axis (Y axis), was focused within a cone on the side-wall of the PCS structure with a rectangular aperture of $50 \times 200 \mu\text{m}^2$ (see Fig. 2a). The angles of incidence within the cone were from 10° to 30° in XZ incidence plane and due to the long rectangular aperture of the beam did not exceed 8° in YZ incidence plane. FTIR measurements were performed with a resolution of 8 cm^{-1} . A gold coated glass slide was used as a 100% reflection reference.

In order to calculate the reflection and transmission spectra, we employed the Fourier modal method in the Scattering Matrix (SM) form [19], [20]. This approach allows the description of the propagation of electromagnetic waves in the multilayer structure, when a few, or even just one, layer is periodic in the X and/or Z directions. For these calculations we used a model in which we considered the structure to be infinitely extended in the X and Y directions and having a finite number of periods along the Z direction, the direction along which the light is incident (see Fig. 4). The SM method

involves splitting the PC slab into elementary planar layers, 95 layers was used in this case, homogeneous in the Y and Z direction and 1D periodic or homogeneous in the X direction. The circular cross section of each pore was approximated by a staircase, consisting of 10 layers. Solutions of Maxwell equations for each layer were found by expansion of the electric and magnetic fields into Floquet-Fourier modes (plane waves). The exact solution was obtained by truncation of the Fourier series to a finite number of plane waves, with $N_g = 29$ [15]. Of course, a real PC structure does not have perfectly smooth internal surfaces. Rayleigh scattering of light off these rough surfaces may significantly reduce the reflection coefficient within the PSB region. Losses due to scattering can be taken into account by introducing a complex refractive index of the material [15], [21], [22], [23]. We used a complex refractive index for silicon of $n_{Si} = 3.42 + ki$ to model this effect.

IV. RESULTS AND DISCUSSION

Experimental and calculated reflection and transmission spectra are shown in Figs. 5 and 6 in relative wavelength units, a/λ . We used refractive index values of $n_{air} = 1$ for the empty trench-defect and $n_{LC} = 1.56$ for the trench-defect filled with the LC. The value of $n_{LC} = 1.56$ corresponds to the average refractive index for the unoriented LC [24]. The thin line shows the reflection spectrum of the ideal structure calculated without accounting for losses (at $k = 0$), while a thick line denotes the spectrum calculated using $k \neq 0$, the grey areas show the PSB regions. We will focus on the first, or lowest, PSB for TE polarization and on the second and third PSBs for TM polarization, where the localized states related to the trench-defect and to the surface states are expected.

The calculated reflection and transmission spectra depend on the pore radius r , the angle of light incidence, θ , and on the imaginary part of the refractive index, k . The pore radius and the angle of incidence of the light can be determined experimentally only approximately, and the imaginary part

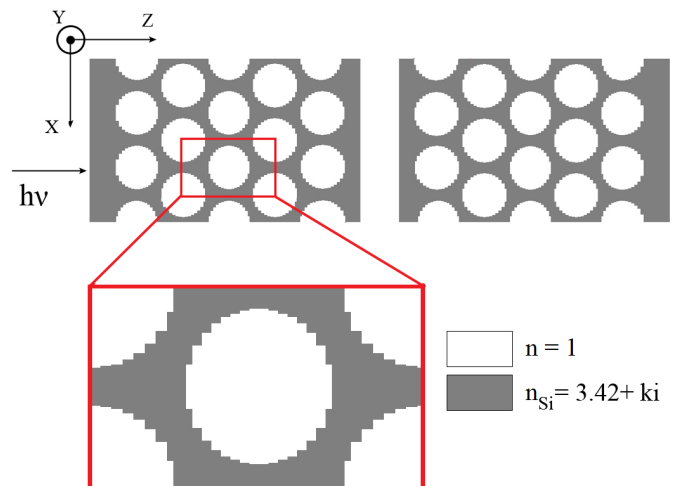


Fig. 4. Two-component model of 2D PC micro-cavity used for calculation of the optical characteristics of the structure by the Scattering Matrix method.

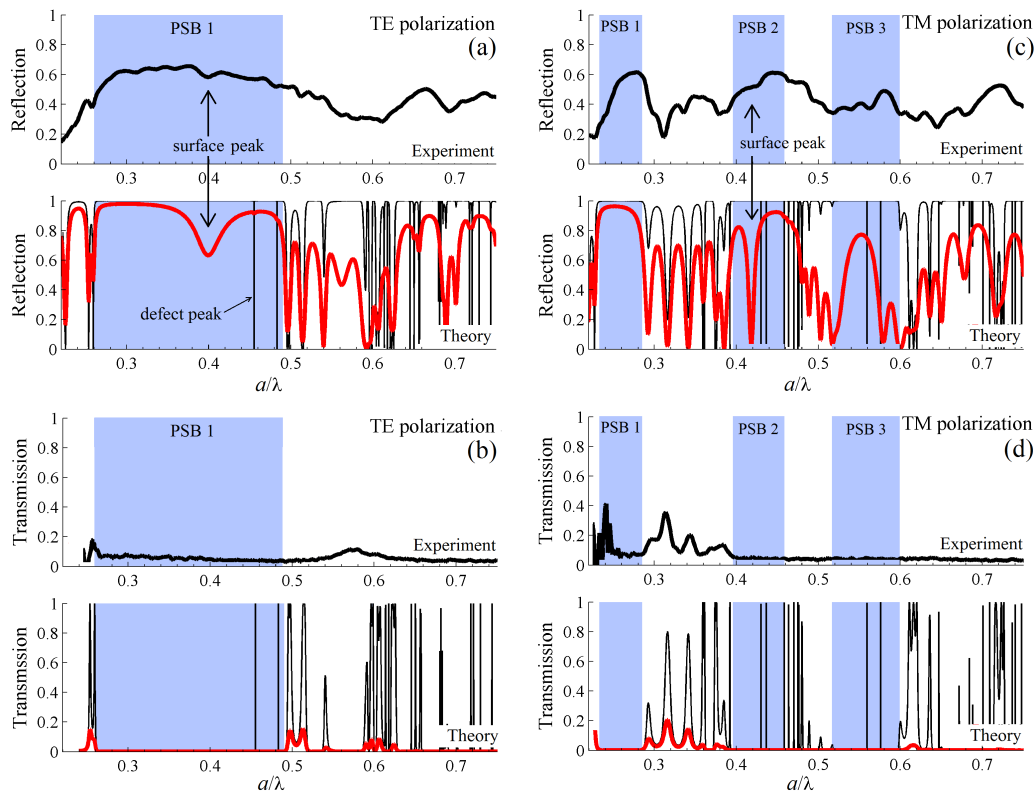


Fig. 5. Experimental and calculated spectra for the sample with an empty trench: (a,c) reflection and (b,d) transmission spectra for (a,b) TE and (c,d) TM polarization. For the calculated spectra, the thin black line corresponds to $k = 0$ and the red line to $k = 0.02$. The filling fraction $r/a = 0.433$, the angle of incidence $\theta = 10^\circ$.

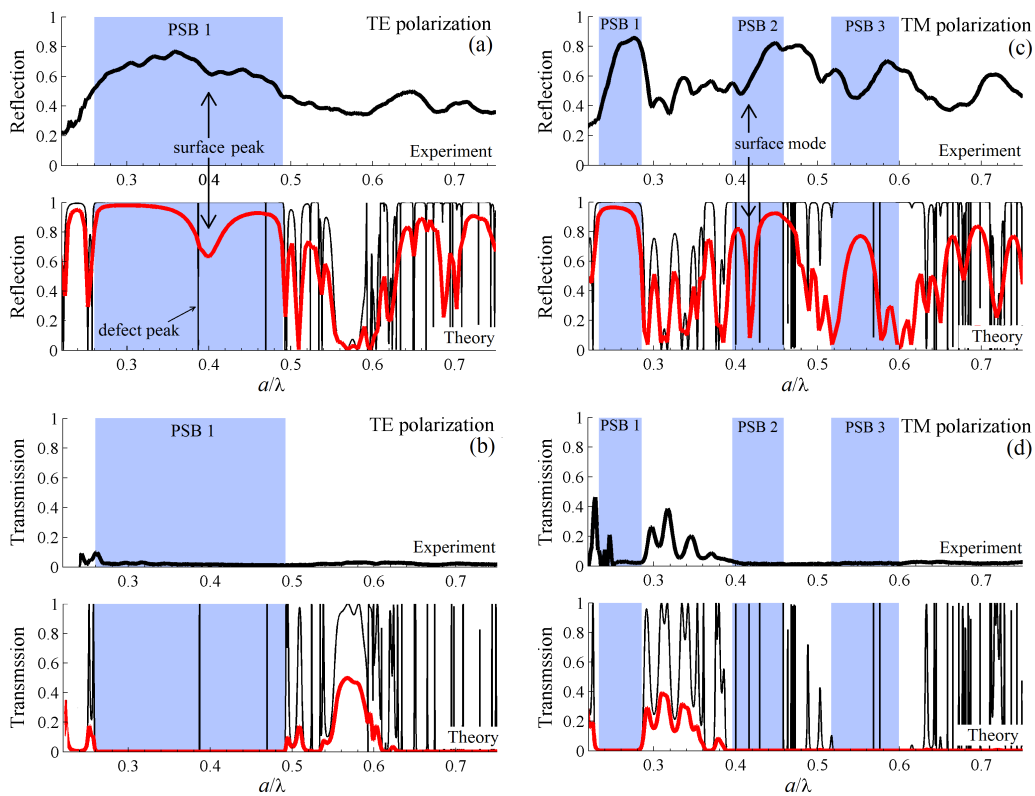


Fig. 6. Experimental and calculated spectra for the sample with a trench-defect infiltrated with the LC: (a, c) reflection and (b, d) transmission spectra for (a, b) TE and (c, d) TM polarization. For the calculated spectra, the thin black line corresponds to calculations at $k = 0$, and the red line to $k = 0.02$. The filling fraction $r/a = 0.433$, the angle of incidence $\theta = 10^\circ$.

of the refractive index cannot be found directly by experiment. Therefore, in order to fit the experimental spectra, these parameters were varied within the following ranges: $r/a = 0.41 - 0.47$, $\theta = 0 - 30^\circ$ and $k = 0 - 0.10$. The experimental and simulated spectra were compared by overlapping of both spectra on the same plot. The selection criteria for the first two parameters were the spectral position of the PSBs and the other spectral extremes. The selection criteria for the extinction coefficient k was a compromise between the amplitude of the surface dip in the reflection spectrum within the PSB, and the amplitude of the Fabry-Pérot oscillations outside the PSB, since an increase in k leads to smoothing of the Fabry-Pérot oscillations and a simultaneous growth in the surface dip amplitude. Best agreement with experiment for both polarizations for an empty trench, as well as for the filled trench, was obtained at $r/a = 0.433$, $k = 0.02$ and $\theta = 10^\circ$. These results coincide well with the average pore radius, as measured by optical microscopy, i.e. $r = 1.6 \pm 0.2 \mu\text{m}$ ($r/a \approx 0.43$).

In accordance with the spectra calculated for the ideal structure without losses, the defect mode shows up as a very narrow line with zero reflection (or 100% transmission) in the minimum. This mode can be seen at $a/\lambda = 0.455$ and $a/\lambda = 0.385$ within the first PSB for TE polarization for the empty and filled trench-defect, respectively. For TM polarization, this trench-defect creates a number of states, represented by narrow lines in the second and third PSB. Peaks at $a/\lambda = 0.4$ (in TE polarization) and at $a/\lambda = 0.42$ (in TM polarization) associated with the surface states have a very small amplitude in the spectra of the idealized structure and, therefore, cannot be seen in the graphs at the scale used here. When $k > 0$, the amplitude of the surface peaks increases significantly, rendering them visible. The surface states are caused by interfacial Si layers, w_1 , at the external borders of the structure. Detailed analysis of these states was performed in Ref. [15]. It has been shown that the near-field electromagnetic field distribution in the vicinity of the interface corresponds to a standing wave, and the mode itself has been assigned to a surface, Tamm-like, state. The spectral position of the surface dips depends on the thickness of the interfacial layers, w_1 , and they can appear within a PSB. Pure PSBs, without surface dips, can be obtained at $0 < w_1 < 0.55a$ in TE polarisation, and at $0 < w_1 < 0.45a$ in TM polarization for $r = 0.45a$. In the micro-cavity structure fabricated here, $w_1 = 2.56 \mu\text{m} = 0.68a$, which means that the surface mode can be observed within the first PSB for the TE polarized incident light. The surface mode can be seen within the second PSB for TM polarization.

In contrast to the surface mode, introduction of the imaginary part to n_{Si} gives rise to the opposite effect on the defect state. The amplitude of the latter peak decreases and its width increases. This results in the very weak peaks both in the experimental and the calculated spectra for $k \neq 0$. Thus, the resonance modes are not seen, and the surface modes dominate within PSBs. Therefore, the resonance peak is practically impossible to detect in our experimental spectra due to scattering losses.

In conclusion we note that due to the fact that not all

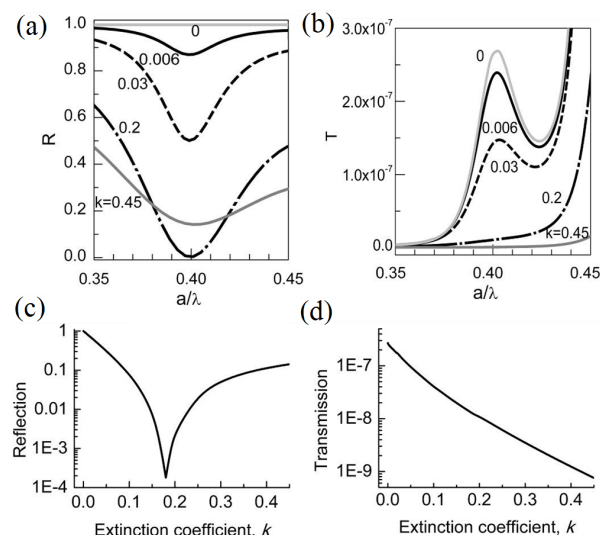


Fig. 7. Influence of scattering losses on the amplitude of the surface peak within the lower PSB for TE polarization of light. The part of (a) reflection and (b) transmission spectra for different values of extinction coefficient k . Dependence on k of (c) the minimal reflection and (d) the maximal transmission at $a/\lambda = 0.4$. The structural parameters are: $r = 0.433a$, $w_1 = 0.683a$, and $w_2 = 0.548a$, the angle of incidence of light $\theta = 10^\circ$.

of the light losses can be accounted for by introduction of the complex refractive index of Si, the observed discrepancy between experimental and simulated spectra particularly for TM polarisation is relatively large. Nevertheless, most of the main spectral features seen in experimental and simulated spectra are in reasonable agreement.

In the next Section we analyze the conditions necessary for the experimental observation of the resonator defect states.

V. THE INFLUENCE OF LOSSES ON THE SURFACE AND RESONANCE MODES

Scattering at the Si-Air or Si-LC interfaces depends on the roughness of the Si surface and on the optical contrast of the refractive indices of the materials located on the both sides of the interface. The surface roughness, in turn, depends on a number of technological parameters [10], [12]. First of all, it depends on the etching current density. The smoothest trench walls can be obtained under anodization at $0.35 < j/j_{PS} < 0.43$, where j_{PS} is the critical current density, corresponding to the transition to the electro-polishing mode [17]. Secondly, the deviation from the design rule, $t \approx a$, leads not only to a significant corrugation of the trench walls, but also to a distortion of the shape and diameter of pores adjacent to the trenches [13]. Roughness can also be reduced by post-anodization treatment, for instance, oxidation or alkaline etching, allowing limited tuning of this property. We can use the extinction coefficient k as a quantitative measure of scattering losses, and evaluate how the amplitude of the surface and resonance peaks depends on k within the first PSB for TE polarization. From Fig. 7a, when losses increase, the amplitude of the surface peak grows, the peak is broadened, and the absolute value of the reflection coefficient in the PSB decreases. The dependence of the minimal reflection

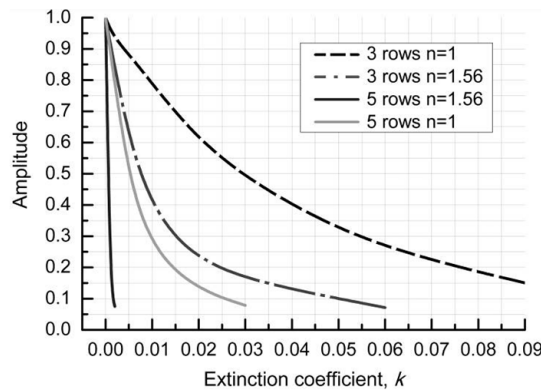


Fig. 8. Calculated dependence of the amplitude of the defect peak within the lower PSB versus k for structures with three or five rows of pores from each side of the trench-defect. For the empty trench, $n = 1$, for the trench infiltrated with the LC, $n = 1.56$. The structure parameters are: $r = 0.433a$, $t_1 = t_2 = t = 0.95a$, $\theta = 0^\circ$, TE polarization of light.

versus the extinction coefficient (Fig. 7c) has a minimum at $k = 0.18$, when an almost total quenching of the reflected signal is achieved. The amplitude of the corresponding peak in the transmission spectrum is extremely small and gradually decreases as k grows (Fig. 7b and d). This explains why the surface peak was not observed in experimental transmission spectra shown in Figs. 5 and 6.

The surface states are characterized by a low quality factor. They may overlap with the defect modes and lead, not only to a reduction of the quality factor of the resulting state, but also completely mask the defect modes. Therefore, in the course of the design of the micro-cavity structure it is necessary to select parameters for which the Tamm states are absent in the PSB. To satisfy this condition we must define suitable values of w_1 and w_2 . As shown in Ref. [15], a similar structure with a filling factor of $r = 0.45a$ and without a trench-defect has no surface states in the lower PSB if $w_1 < 0.55a$. This dictates a requirement of $t_{1,2} < a$. This technological restriction is expressed as $t_{1,2} = 1.13a - 0.95a$ [10], [12]. This means that the absence of surface dips within a PSB does not prevent the fabrication of a good quality microcavity structure using the described technology. Let us consider a resonator structure, in which the distance from the centre of technological and defect trenches to the nearest row of pores, inside and outside the structure, are equal, i.e. $t_1 = t_2 = t$. Our calculations show that, if $t \leq a$, then in the range of filling factors $r = 0.41a - 0.47a$, the surface peak is absent in the first PSB for TE polarization. Let us then estimate how large the influence of light scattering on the amplitude of the defect mode is. For this, we consider the dependence of the amplitude versus the imaginary part of the silicon refractive index. Figure 8 shows the defect peak amplitude versus k for structures with 3 and 5 periods from each side of the trench-defect.

It can be seen that the amplitude of the defect peak is reduced when the losses increase. For a smaller number of pore rows, the amplitude of the defect-peak is less sensitive to the scattering losses. LC infiltration leads to a sharper decline in the amplitude of the defect peak. A comparison of the experimental and calculated spectra in Fig. 5 and 6 shows that

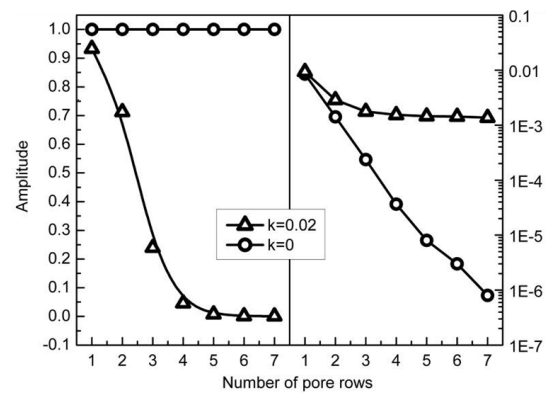


Fig. 9. Dependence of amplitude (left panel) and width (right panel) of the defect peak on the number of periods on both sides of the trench-defect, infiltrated with LC ($n = 1.56$) for ideal (circles) and real (triangles) structures. The structural parameters are: $r = 0.433a$, $t = t_1 = t_2 = 0.95a$, $\theta = 0^\circ$, TE polarization of light was used.

light scattering in the fabricated structures can be estimated as $k = 0.02$. With this value for losses, the amplitude of the resonant peak for the structure with three rows of pores would have been up to $\sim 60\%$ of the total reflection for an empty trench-defect and up to $\sim 24\%$ for a trench filled with LC. In structures with a greater number of periods, the defect mode has an even smaller amplitude.

Now let us estimate how many rows of pores are required in a structure with an LC filled defect (at $n = 1.56$) in order to obtain a cavity with a significant dip within the PSB using existing technology. To do this, we calculate reflection spectra for the structure as we vary the number of rows of pores on each side of the trench-defect from one to seven. Next, we determine the amplitude of the resonance dip and the Full Width at Half-Maximum (FWHM) of the amplitude from these reflection spectra. From Fig. 9, the amplitude and FWHM of the dip for the ideal structure ($k = 0$) demonstrates predictable behavior as the number of structure periods increases. The dip amplitude is constant and equal to 1, and the FWHM decreases with the number of pores. When $k \neq 0$ the behaviour of these parameters is more complex. As the number of pore rows increases, both the amplitude and FWHM of the dip decrease. For a structure, consisting of two rows of pores, the amplitude is $\sim 72\%$ of the total reflection at a quality factor, $Q = \omega/\Delta\omega \approx 134$. For a structure with three rows of pores, the amplitude drops to $\sim 24\%$, and the quality factor increases to $Q \approx 220$. When the number of pore rows is greater than three, the amplitude of the resonance dip drops to less than 10%. Thus, we conclude that the number of pore rows on each side of the trench-defect should be ≤ 3 .

The fabrication of a micro-cavity with such a small number of periods in the structure described above is extremely difficult, due to the low mechanical strength of the narrowest part of the structure. Use of more complex technology, leaving the PC layer on the Si substrate, will interfere with optical measurements as the substrate will partially block the converging light beam projected on the side-wall of the structure. In other words, the design of the micro-cavity should take account of how the light is to enter the structure. Note that

the micro-cavity based on macro-porous silicon with a defect present in the waveguide, a missed row of pores, has two pore rows on both sides of the defect [25]. It was found experimentally that the quality factor of one of the defect states was 190. In our earlier work, we successfully fabricated micro-cavity structures with a lattice period of $8\ \mu\text{m}$ and three periods. Unfortunately, the lower PSB of these structures is outside the spectral range of our instrument. This structure would be expected to find application in the far-infrared range ($\lambda = 16 - 33\ \mu\text{m}$).

VI. CONCLUSION

We conclude that a tunable micro-cavity can be fabricated by joint photo-electrochemical etching of macropores and trenches in silicon. However, to avoid the appearance of surface modes within PSBs, only thin layers of w_1 and w_2 are acceptable. These layers can be obtained by specifying $t_{1,2} \leq a$ in the lithographic mask and $r/a \geq 0.41$. Also, scattering losses must be minimized in order to obtain a reasonable amplitude and quality factor. Using current technology, in which scattering losses are characterised by $k = 0.02$, the number of pore rows on both sides of the trench-defect should be no more than three.

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