Dispersion relation of 3D photonic crystals based on macroporous silicon

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ABSTRACT

Extended 3D photonic crystals based on macroporous silicon are prepared by applying a periodic variation of the illumination during photoelectrochemical etching. If the lateral pore arrangement is 2D hexagonal, the resulting structure exhibits a simple 3D hexagonal symmetry. The dispersion relation along the pore axis is investigated by optical transmission measurements. Photonic band gaps originating from the pore diameter modulation are observed and the group velocities of the photonic bands are determined by analyzing the Fabry-Perot resonances. Furthermore, angular resolved transmission measurements show a spectral region of omnidirectional total reflectivity.

INTRODUCTION

2D macroporous silicon photonic crystals have been extensively studied in the last seven years since the pioneering work of Lehmann and Grüning [1,2]. A recent review is given by Schilling et al. [3]. The concept to obtain 3D photonic crystal by pore diameter modulation has already been predicted seven years ago [4], but just recently we have shown the first realizations of these 3D photonic crystals [5]. In the following we are going to analyze the optical properties in detail.

FABRICATION OF THE 3D PHOTONIC CRYSTALS

The fabrication of 2D macroporous silicon photonic crystal is described in Refs. 1-4. The pattern and the pitch of the 2D pore array are defined by lithographic prestructuring. The pore radius is determined by the etch current and can therefore be controlled by the backside illumination. Increasing the illumination of the sample causes a higher hole generation rate. This results in an increased total current density $j$ leading to a higher porosity and a larger radius of the pores. To achieve a periodic variation of the pore diameter with pore depth, the illumination intensity and thus the etch current is varied periodically during pore growth. Figure 1 shows examples of resulting structures. The macropores are initially arranged in a 2D hexagonal lattice with a pitch of $a = 1.5 \, \mu m$ (figure 1e). The etch parameters are: $c_{HF} = 4 \, \text{wt}\%; T = 17^\circ\text{C}; U = 1.5 \, V$. The illumination of the wafer backside was modulated applying zig-zag profiles with different periods. Shorter modulation periods of the illumination lead to shorter periods of the pore diameter modulation. Although the measured etch current exactly follows the intended zig-zag profile, the etched pore profiles show a slightly smoother shape. Especially for the shortest shown modulation period the minima and maxima of the zig-zag current profile are smeared out and the amplitude of the pore diameter modulation is reduced.
Figure 1. a)-d) SEM-images of cross sections of four different samples with different modulation periods $l_z$. e) Top view revealing the 2D hexagonal (triangular) ordering of the pores and the pore shape. f) 3D hexagonal Brillouin zone of the resulting simple 3D hexagonal photonic crystal assuming circular pores.
OPTICAL PROPERTIES

Assuming a circular pore cross section and a sinusoidal modulation of the pore radius \( r \) with 
\[ r = r_0 + \Delta r \sin \left( \frac{2\pi z}{l_z} \right), \]
the structure possesses a simple 3D hexagonal symmetry. The first Brillouin zone is shown in figure 1f. However, thorough analysis of figure 1e suggests that the pore form is not perfectly round but resembles more like squares with rounded edges. This squareness leads to a reduction of symmetry of the photonic crystal and a splitting of originally degenerate photonic bands [6]. Nevertheless, for the sake of simplicity, we assume in the following that the pores are circular which is a good approximation of the complete analysis [6].

![Graph](https://via.placeholder.com/150)

**Figure 2.** Transmission along pore axis (Γ-A direction) for a structure with \( a = 1.5\mu m, l_z = 2\mu m, r_0 = 0.62 \mu m, \Delta r = 0.09 \mu m \). Left: calculation applying a 1D effective refractive index model; centre: transmission measurement; right: section of 3D band structure calculation.

![Graph](https://via.placeholder.com/150)

**Figure 3.** Left: 3D band structure for a modulated pore structure with \( l_z/a = 0.55, r/a = 0.42 \) and \( \Delta r/a = 0.06 \). Right: normalised density of photonic states.

The dispersion relation for light propagating along the pore axis (Γ-A direction) is governed by the modulation period of the pore diameter. Therefore, optical transmission measurements with normal incidence were performed (figure 2, centre). Two spectral regions of vanishing transmission are observed as indicated by the gray bars. These regions are in good agreement with the first and second order bandgaps in the Γ-A section of the 3D band structure. The
transmission along the pore axis can also be calculated approximating the structure by a 1D model. The structure was divided into several thin layers stacked in z-direction. For each of these layers an effective refractive index is calculated applying the Maxwell-Garnet formula. The transmission for this model is analytically calculated by the transfer matrix method (figure 2 left). The spectral range of the vanishing transmission around 1250 cm\(^{-1}\) coincides very well with the first order band gap observed in the 3D calculation and in the transmission measurement. However, the second order bandgap at 2250 cm\(^{-1}\) is shifted to higher frequencies in the 1D transmission calculation. This indicates that at higher frequencies the Maxwell-Garnet formula fails. The lateral periodicity of the refractive index in the xy-plane can no longer be neglected. To investigate if the structure might exhibit a complete 3D photonic bandgap, the band structure for a photonic crystal with the parameters \(l/a = 0.55\), \(r/a = 0.42\) and \(\Delta r/a = 0.06\) was calculated (figure 3). In this case, the bandgap in the \(\Gamma\)-M-K-plane overlaps with the first order gap at the \(A\)-point. However, a complete 3D band gap does not exist since near the H and L points, as well as at the \(\Gamma\)-point photonic bands cross this spectral region. Even widening of the pores to \(r/a > 0.5\) at places with maximum pore radius would not yield a complete 3D photonic bandgap. Nevertheless, a reduction of the photonic density of states by 50\% is theoretically possible (figure 3).

\[\text{Fig. 4: Comparison of the experimentally determined group velocity with that obtained from 3D band structure calculations for the structure from Fig. 2.}\]

Besides the position of the band gaps, the transmission measurements along the pore axis contain also information about the dispersion relation of the photonic bands in the \(\Gamma-A\) direction. Below and above the first order bandgap, the transmission curves exhibits pronounced oscillations (figure 2). These are Fabry-Perot resonances, which are caused by multiple reflections of the light between the surface air/photonic crystal and the interface photonic crystal/bulk silicon substrate. The spacing between neighboring Fabry-Perot resonances in the k-space \(\Delta k_{\text{max}}\) and in the frequency space \(\Delta \omega_{\text{max}}\) of the photonic crystal read

\[
\Delta k_{\text{max}} = \frac{\pi}{d}; \Delta \omega_{\text{max}} \approx \frac{\partial \omega}{\partial k} \Delta k_{\text{max}} \quad (1)
\]

where \(d\) describes the pore depth or the thickness of the photonic crystal. Merging these two relations, the dispersion relation in \(\Gamma-A\) direction of the photonic bands can be obtained purely from the experimentally determined values \(\Delta \omega_{\text{max}}\) and \(d\). The group velocity \(v_g\) along \(\Gamma-A\) is the derivative of \(\omega\) with respect to \(k_{\Gamma-A}\)

\[
v_g = \frac{\partial \omega}{\partial k_{\Gamma-A}} \approx \Delta \omega_{\text{max}} \frac{d}{\pi} \quad (2)
\]
Figure 4 shows a comparison of the experimentally determined and the calculated group velocities. The latter one has been obtained by taking the derivative $\partial \omega / \partial k$ of the photonic bands in the band structure in figure 2. Good agreement between theory and experiment is observed. The group velocity decreases near the first order photonic band gap around 1250 cm$^{-1}$, as expected. Further optical properties of this 3D photonic crystal can be revealed performing angular resolved transmission measurements. To select those modes of the photonic crystal which can couple to outside radiation incident from the top surface (Γ-A surface), the light cone has to be considered. The light cone corresponds to an angle of incidence of $\alpha = 90^\circ$ from the Γ-A direction (dashed oblique lines in figure 5). All modes of the photonic band structure which lie below the light cone in the gray shaded area are “bound” modes. They can not be excited by radiation incident from the Γ-A surface under any angle. Only the white part of the band structure is of interest. Thorough inspection reveals a spectral range (indicated by the horizontal dashed bar) with no photonic bands in the white region. No photonic crystal modes are available which could be excited by incident radiation. All the radiation incident to the top Γ-A surface with frequencies in this range should therefore be totally reflected. This is called omnidirectional total reflection [7]. To verify this experimentally, transmission measurements were performed for angles of incidence $\alpha = 0^\circ$ and $\alpha = 70^\circ$. The sample was tilted towards the Γ-M and the Γ-K direction and s- and p-polarization were separately measured. Figure 6 shows exemplarily the transmission for a tilt towards the Γ-M direction. In the range 1300 cm$^{-1} < \omega < 1380$ cm$^{-1}$ all transmission spectra show vanishing transmission corresponding to total reflection. This spectral region represents the overlap of the band gaps for the radiation incident under $\alpha = 0^\circ$ and $\alpha = 70^\circ$. It agrees very well with the horizontal dashed bar indicating the spectral range of omnidirectional total reflection. Strictly speaking these experimental results confirm only total reflection for incidence angles $0^\circ < \alpha < 70^\circ$. However, the transmission curves for grazing incidence ($\alpha = 90^\circ$) will not differ significantly from the ones with $\alpha = 70^\circ$ as can be seen from the intersections of the incidence lines for $\alpha = 90^\circ$ (light cone) and $\alpha = 70^\circ$ with the second photonic band. Compared to the intersection of the incidence line for $\alpha = 70^\circ$ with the second band, there is a shift of 1.6% to lower frequencies. Taking this small shift into account, a region of omnidirectional total reflection between 1321 cm$^{-1} < \omega < 1380$ cm$^{-1}$ with a spectral width of $\Delta \omega / \omega = 4.4\%$ has been determined experimentally.

Figure 5. 3D band structure for a structure with $l_z/a = 1.33$, $t/a = 0.42$ and $\Delta r/a = 0.06$. The oblique dashed lines represent the light cone. The gray shaded area below contains the photonic modes bound to the photonic crystal. They can not couple to the incident radiation. The horizontal dashed bar indicates the spectral range of omnidirectional total reflection.
CONCLUSION

3D photonic crystals based on macroporous silicon have been fabricated by periodical variation of the pore diameter with the pore depth. This was achieved by periodic modulation of the illumination intensity during the photoelectrochemical pore etching process. Transmission measurements along the pore axis revealed photonic bandgaps which originate from the pore diameter modulation. By analysis of the Fabry-Perot resonances in the transmission curves the group velocity along the Γ-A direction for the lower bands could be determined. Angular resolved transmission measurements show that the modulated pore structure act as omnidirectional reflector in very good agreement with theory.

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REFERENCES