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PAPER

Bandgap widening in macroporous silicon photonic crystals by multiperiodic structures

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**Keywords:** spectroscopic gas sensing, macroporous silicon, photonic bandgap, 3D photonic crystals, multiperiodic photonic crystals**Abstract**

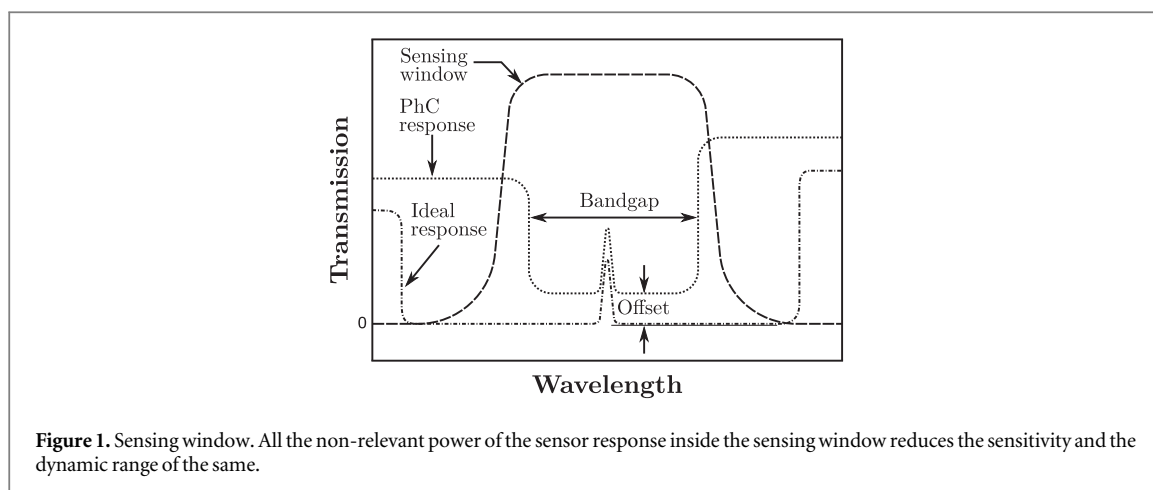
Large bandgaps with low transmission in 3D macroporous silicon photonic crystals have been proved as an interesting technology for the development of optical filters and spectroscopic MIR gas sensors. The aim of this study is the investigation of different bandgap widening methods based on multiperiodic structures for 3D macroporous silicon photonic crystals. To do so, chirped modulations and structures with different periodicity groups have been modelled and theoretically analysed by means of 3D FDTD simulations. They have revealed that by using different decreasing periodicity groups, bandgaps with null transmission and widths as high as 1800 nm, 4 times the original single periodicity photonic crystal bandgap, can be obtained. Furthermore, it has been shown that a resonant cavity with a 20% transmission can be placed in a 1 μm wide bandgap. The results open a way to use this type of structures not only for gas sensing but also for other purposes such as wide stop-band filters, selective filters or broadband mirrors.

Introduction

Photonic crystals (PhCs) are structures with periodical alternation of the refractive index. This periodicity results in frequency dependent constructive and destructive interferences when light travels through them, which confers special properties to PhCs. Among other optical properties, the PhCs present bands of frequencies in which light propagation within the structure of the PhC is completely forbidden—the so called photonic bandgaps—[1]. By introducing defects in the lattice, i.e. breaking the periodicity of the PhC, resonant cavities can be created [1], permitting the propagation of light in a narrow range of wavelengths inside the bandgap. In that sense, the bandgap itself can be considered as a band-stop filter but when the resonant cavity is present, it gives place to a narrow band selective filter in transmission.

The extraordinary optical properties of the PhCs have enabled their application in different fields: biochemical sensing [2], signal processing [3] or lasing [4]. In order to optimize the performance of the PhCs for a given application, the topology of the PhC may be tailored. In our case, we are especially interested in obtaining PhCs with wide enough bandgaps that enable the fabrication of optical filters and compact spectroscopic gas sensors in the mid infrared region (MIR)—wavelength region between 4 μm and 8 μm , where gases such as CO₂, NO or CO exhibit important absorption.

In the proposed gas sensing application, the light comes from a broadband MIR light source and perpendicularly impinges on a PhC with an embedded resonant cavity whose resonant wavelength is centred at a fingerprint of a target gas. After them, a gas cell and a photodetector are used to obtain the gas absorption at that wavelength [5]. Further research has still to demonstrate whether placing the PhC inside the gas cell could help to increase the interaction pathlength between light and gas, similarly to the gas sensor reported by Wehrspohn *et al* [6].



The response of the PhC inside the sensing window, the frequency range of working frequencies of the source and the photodetector combination, all are of crucial importance in order to achieve better performance of a final device. As it can be seen in figure 1, the non-relevant transmitted power in the sensing window saturates the photodetector and reduces the sensitivity and the dynamic range of the sensing device. To optimize the optical figures of the final device, all the received power in the sensing window must contain useful information of the gas absorption—ideal case in figure 1. Additionally, the width of the bandgaps has a direct impact in the cost of the sensor system; while producing macroporous structures with narrow transmission bands practically does not increase fabrication costs, narrow spectrum sources and narrow spectral range photodetectors are usually more expensive than broadband ones. Then, the use of macroporous PhCs as filter allows to reduce the requirements of source and photodetector.

In order to increase the sensitivity and the noise to signal ratio of the spectroscopic sensor, the PhC bandgap must be wider than the wavelength working range of a MIR source–photodetector combination, while transmission in the resonant peak must be maximum. From our experience with commercial light sources [7] and detectors [8] for gas sensing in the infrared, we estimate that a bandgap width of around 1 μm would be appropriate in most cases.

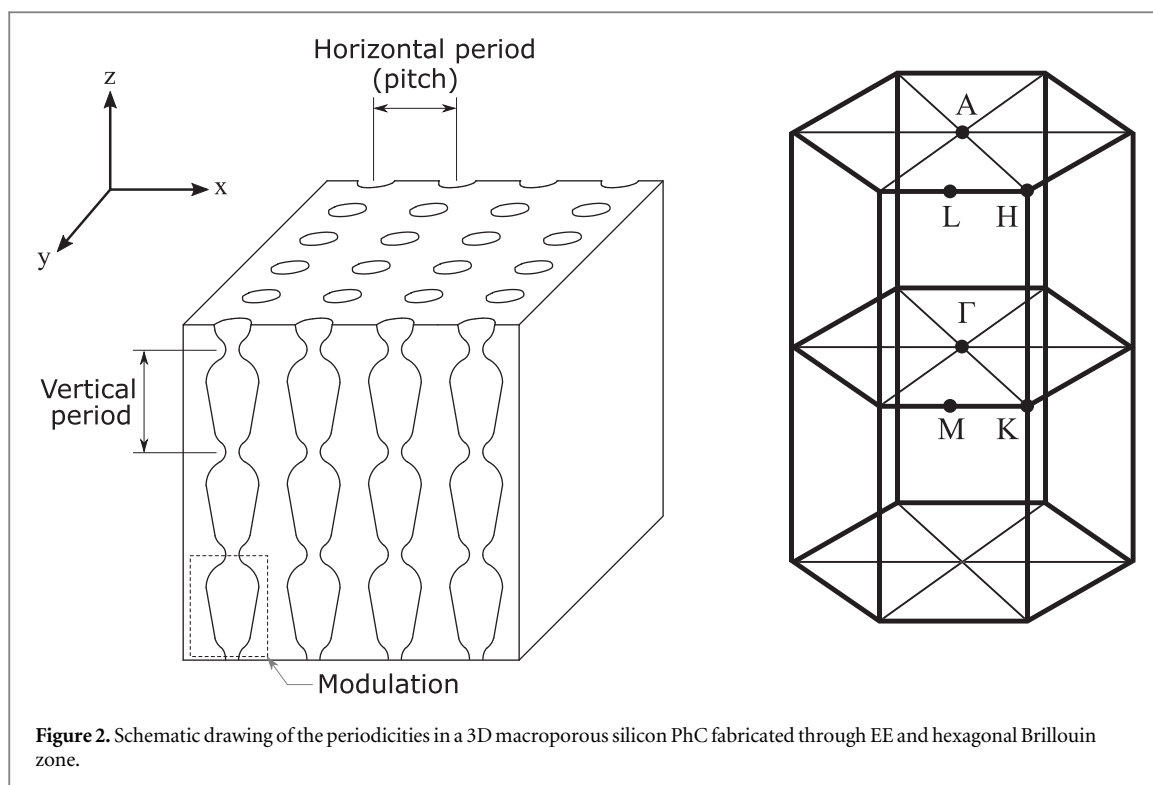
Electrochemical etching (EE), the fabrication method used in this work, is a low-cost and repeatable process that allows obtaining in a single etching step the multiple pores that conform the PhC. Therefore, the sequential deposit of multiple layers, which becomes expensive and introduces layer roughness and thickness deviations that reduce the performance of other similar 1D PhCs [9], is avoided. Moreover, the fabrication costs are reduced and a high throughput is possible.

EE permits the etching of air pores in silicon by dissolving the silicon in a hydrofluoric electrolyte solution [10]. In addition, by modifying the conditions of the etching, the shape of the pores can be modulated [11], resulting in a concatenation of air modulations in bulk silicon which form a 3D PhC—see figure 2. The distribution of the pores follows a horizontal square lattice and a vertical periodic modulation, which define the wavelength working range. For this work, we have simulated macroporous silicon PhCs with a 700 nm horizontal periodicity and a 900–1500 nm vertical periodicity, which results in bandgaps centred between 4 μm and 8 μm , region that includes the MIR gas fingerprints of different gases of interest.

This technology presents certain intrinsic advantages such as the fact of working with crystalline silicon, with very low losses in the MIR region and a relatively high refractive index contrast between air and silicon which allows to obtain wide bandgaps. Furthermore, the pores are open, enabling the interaction of the confined light with the pore filling.

In this study light with perpendicular incidence, following the Γ –A pore’s growth direction—see figure 2, has been chosen because the alignment between source, PhC and detector is easy and the optical response is independent of the polarization. Moreover, the fabrication method, electrochemical etching, produces pores in the direction transversal to the surface of the sample. Thus, our interest is to obtain wide bandgaps in this particular configuration.

Different research groups have dealt with the bandgap widening of PhCs, usually facing the problem with a theoretical approach. Efforts have been put to improve the width of the forbidden band in 2D PhCs. Men *et al* [12, 13] studied the modification of the shape of the modulations and the lattice distribution, and Cox and Dobson [14] investigated the effect of the refractive indexes of the used materials in the bandgap. Similarly, Men *et al* [15] also theoretically proposed novel lattice distributions in 3D PhC. However, although with some of the proposed topology variations the obtained bandgaps are remarkably widened, $\Delta\omega/\omega$ (%) \approx 25—see



diamond-2 topology in [15]—, the optimal lattices and modulation shapes result in very complicated or impossible fabrication [13, 15].

Multiperiodic structures—also called photonic heterostructures—with double or triple periodicity—binary and ternary PhCs—are a hot topic in PhCs [16]. Among other properties, they can be used for bandgap enlargement, for instance of 1D PhCs in reflexion [17–19]. In a similar approach, the chirped structures have also been used to widen the bandgaps, some examples are 1D PhCs Bragg chirped reflectors [20], the use of chirped microporous 1D reflectors for solar cells [21] and chirped macroporous silicon PhCs working in thermal emission [22].

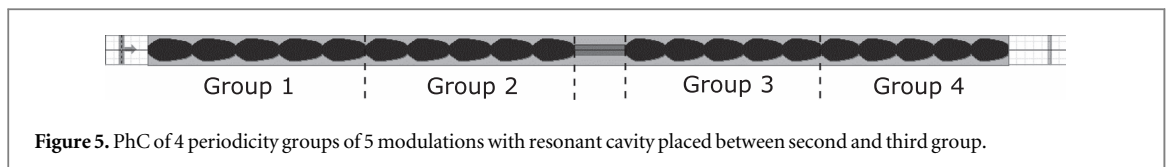
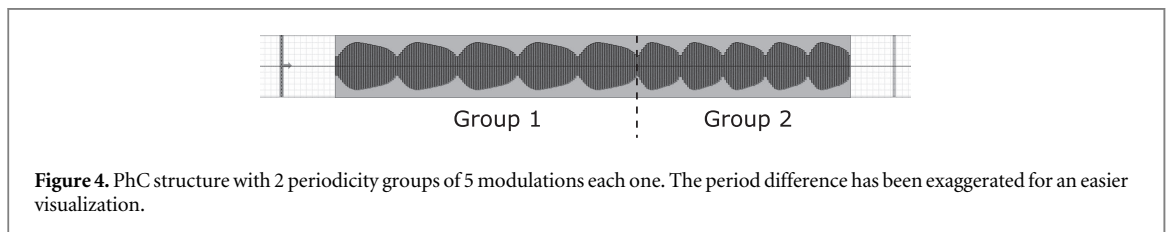
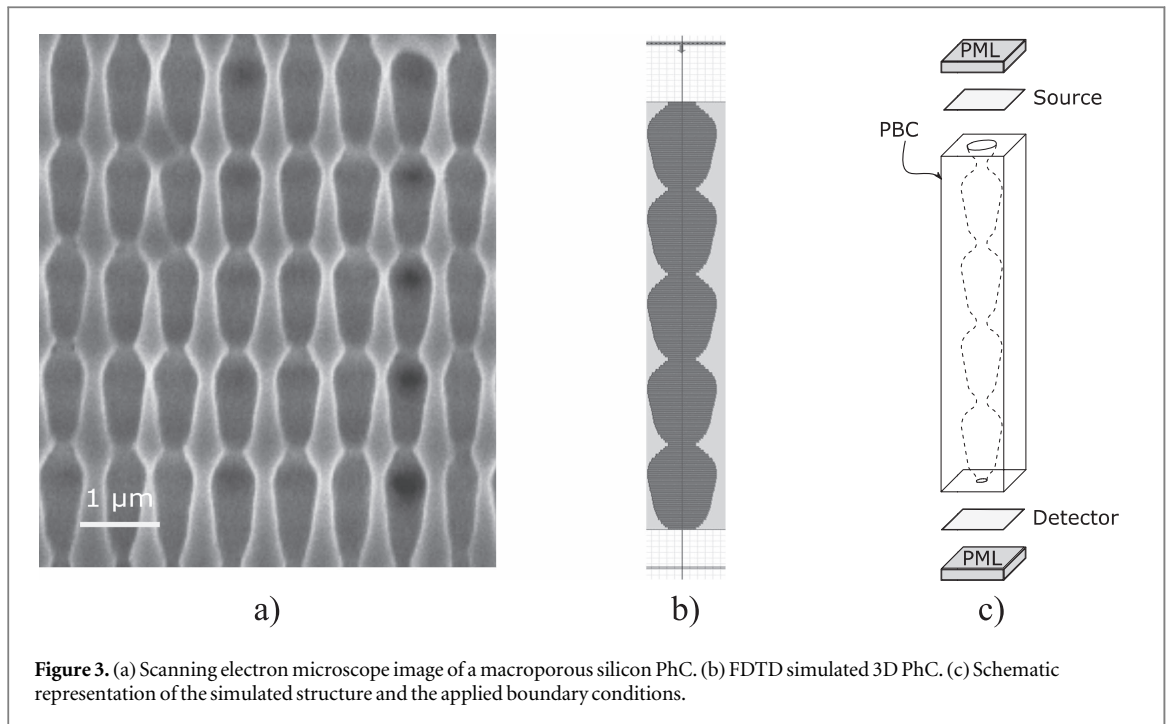
In addition to completely chirped structures, here we also investigate the use of two and four clearly contrasted periods as a technique to enlarge the bandgap of the macroporous 3D PhCs in transmission. The idea behind this strategy is the concatenation of the multiple bandgaps provided by PhCs with different periodicity. However, in this case there is not a repeatability of a structure with different periods in the PhC as in the most typical binary and ternary PhCs [17–19] but there are periodicity groups located in series, similarly to a hybrid between classical heterostructures and chirped PhCs. Finally, a resonant cavity has been introduced to observe the effect of a multiperiodic structure with wide bandgap in the optical response, transmission and quality of the cavity.

Simulation

All the proposed strategies to widen the bandgap—PhC structures with two periodicities, four periodicities and completely chirped structure—have been simulated using a 3D finite difference time domain (FDTD) simulation software. The optical transmission spectra of the PhC structures have been obtained, looking carefully at the transmission inside the bandgap—also called offset in this work; see figure 1—and the bandgap width, defined as the 10% rise from the stopband level.

The fabrication constrains are considered by simulating vertical periods longer than the limiting horizontal pitch [23] and by using a realistic model obtained from SEM images of previously fabricated pores [24]—see figure 3(a). Figure 3(b) shows a vertical cut of the simulated pore passing through its revolution axis.

The performed simulations of the pores do not consider bulk silicon underneath the porosified region. In practice, the porosification of silicon samples does not need to be done in the whole thickness of the silicon sample, often it is done until the pores arrive to a given length. Unporosified silicon can be removed or thinned to the desired thickness. Hence, the simulated region represents a membrane with pores extending from side to side. In order to define a 3D square periodic lattice, periodic boundary conditions (PBC) have been set parallel to the axis of the pore growth—see figure 3(c) and perfect matching layers (PML) have been set after and before the



source and the detector. A Gaussian modulated continuous wave light source is set to emit in the pore's direction Γ -A—see figure 2. After the PhC pore, a detector is placed to obtain the transmission spectrum, which is normalized to the source emission. The grid resolution used in simulations is 10 nm.

The first simulated structure has been previously reported [25], it consists of a PhC with five modulations with single period, 900 nm in our reference case—see figure 3(b). Then, the different widening techniques have been analysed: the use of two periodicity groups see—figure 4, four periodicity groups and chirped modulations. We refer as periodicity group to a number of modulations with exactly the same period.

Finally, a PhC with four periodicity groups and a resonant cavity inserted in the middle of the structure has been simulated. The cavity is a straight cylinder of 1.20 μm length and a diameter of 0.23 μm located between the second and the third group. The structure is represented in figure 5.

Results and discussion

A PhC with 5 modulations and single vertical modulation period—see figure 3(b) has been simulated with period values ranging from 900 nm to 1200 nm. The evolution of transmission spectra is depicted in figure 6(a). The effect of the number of modulations in the spectral response of a single periodicity PhC has also been studied in our 900 nm reference case, it can be observed in figure 6(b). As it can be seen, the bandgap of the structure with 5 modulations and 900 nm vertical period, used as reference, presents a 10.9% bandgap transmission and 478 nm width.

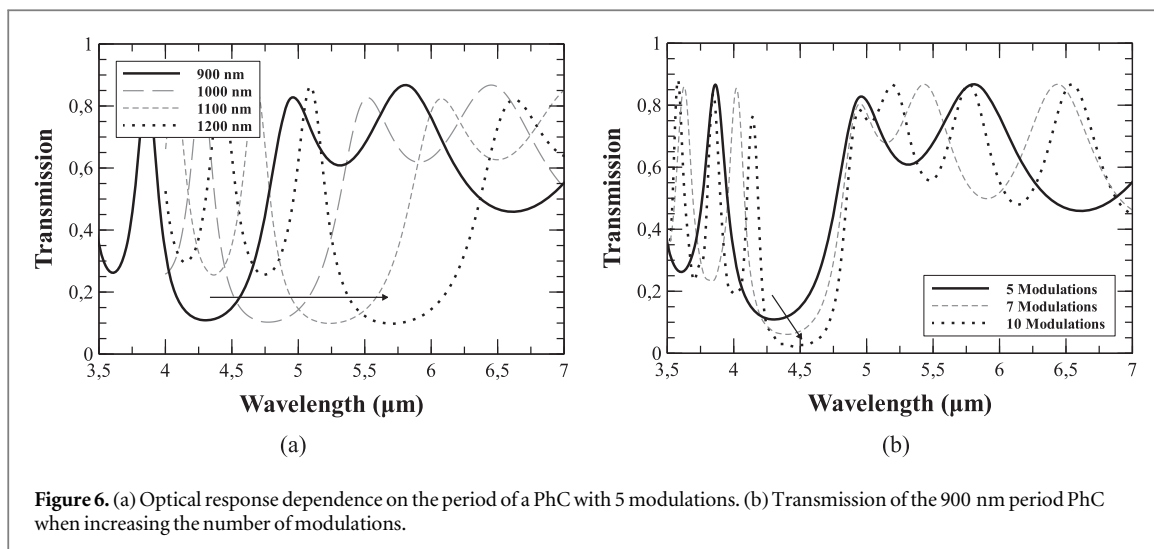


Figure 6. (a) Optical response dependence on the period of a PhC with 5 modulations. (b) Transmission of the 900 nm period PhC when increasing the number of modulations.

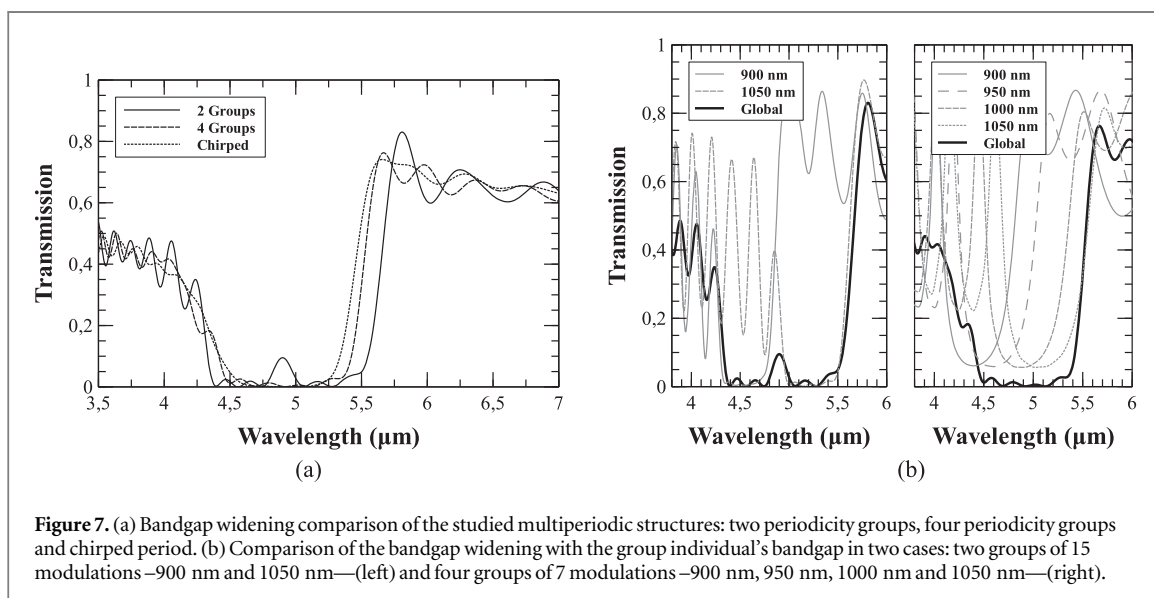


Figure 7. (a) Bandgap widening comparison of the studied multiperiodic structures: two periodicity groups, four periodicity groups and chirped period. (b) Comparison of the bandgap widening with the group individual's bandgap in two cases: two groups of 15 modulations –900 nm and 1050 nm—(left) and four groups of 7 modulations –900 nm, 950 nm, 1000 nm and 1050 nm—(right).

In a PhC with a single periodicity, the obtained bandgap width is far from the $1 \mu\text{m}$ desired values. It slightly increases in PhCs with longer periods but the achieved bandgap widening is not sufficient for our purposes. Moreover, for longer periods, the bandgap moves away from the MIR region of the gas fingerprints.

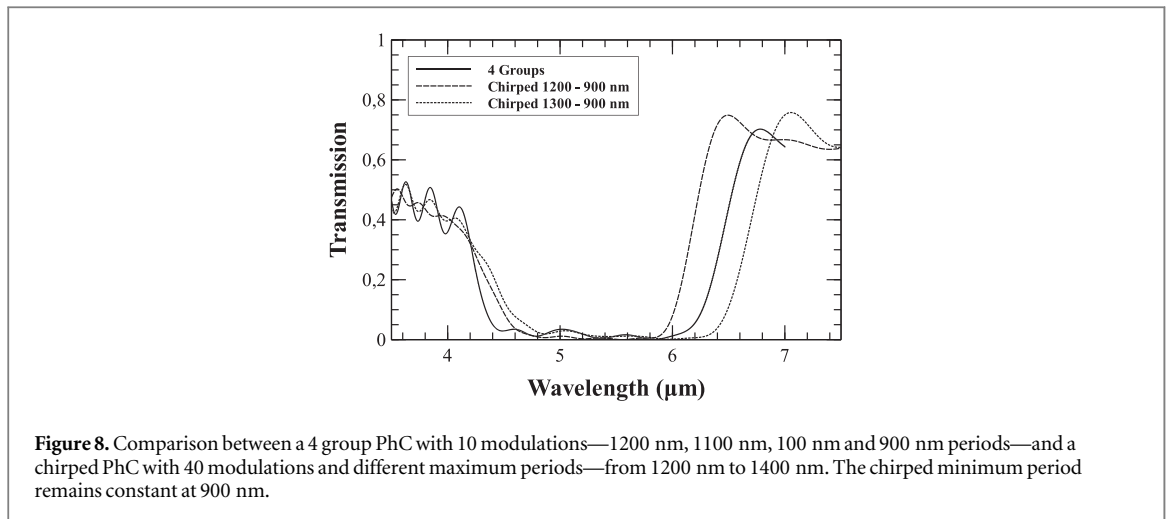
It can be observed that when 5 modulations are used, the transmission in the bandgap is approximately 10%. As suggested in previous works [1, 18], the offset can be reduced by adding modulations. Figure 6(b) shows that this mechanism also proves to be efficient in macroporous PhCs: the addition of 5 modulations reduces the offset from 10.9% to 2.2%. This phenomenon can be explained by the reflection that occurs in each interface between modulations, especially strong in the bandgap area. Then, more modulations imply a higher total reflection.

Finally, it can be observed that the slope of the bandgap edges is steeper with the increase in the number of modulations. This result can be useful for signal processing, where the desired cut-off frequencies should be as abrupt as possible.

Bandgap widening by multiperiodic structures

As described previously, two periodicity groups, four periodicity groups and chirped modulations have been studied to determine which type of structure is more appropriate to widen the bandgap.

Figure 7(a) is a comparison of the transmission spectra of the different multiperiodic proposed structures having a similar number of modulations and the same maximum and minimum vertical periodicity, 1050 nm and 900 nm respectively. The structure with two groups consists of 15 modulations of 1050 nm and 15 modulations of 900 nm. The one with four groups, consists of 7 modulations of 1050 nm, 1000 nm, 950 nm and 900 nm. In the case of the chirped structure, the period decreases linearly from 1050 nm to 900 nm in 30 steps.



From the results shown in figure 7(a), and comparing them with those shown in figure 6, it can be said that the transmission bandgap can be effectively widened by using multiperiodic structures, achieving near $1 \mu\text{m}$ widths and null bandgap transmission. Nevertheless, there are important differences between the used techniques. The bandgap is reduced when the number of groups is increased, being the chirped modulation—the extreme structure in which each group has only one modulation—the one with narrowest bandgap. Moreover, if the PhC has the same total modulations, the fewer the groups introduced, the steeper the edges of the bandgap. More groups also imply a smoother response, inside and outside the bandgap.

However, although the widest bandgap is achieved with the lowest possible number of groups, if the period of these groups are too separated, a transmission region appears in the middle of the bandgap—see two groups case in figures 7(a), (b). This undesired effect is due to the incomplete overlapping of individual bandgaps, which in our case occurs when the period of the groups differs in more than 100 nm. It can be solved by adding groups whose bandgap covers the non-overlapping region—see 4 groups in figures 7(a), (b).

In figure 7(b) it can be seen that the overlapping of bandgaps critically depends on the individual bandgaps of the groups. When the groups consist of a reduced number of modulations, as in the case of four groups or chirped modulation, the groups' individual bandgap have some bandgap transmission and smoother edges. The fact of having edges that are more gradual facilitates the overlapping of individual bandgaps. Nonetheless, it results in an increased transmission near the global PhC edges' range of frequencies, which is not covered by other individual bandgaps, reducing the effective bandgap of the multiperiodic PhC.

Moreover, as explained before, the fact of introducing more groups increases the smoothness of the response. When light travels thorough different groups, there is an effective averaging of their individual spectra. Then, more groups with different periodicities increase the averaging, reducing the effect of the individual interference patterns that can be seen in a group with a single periodicity. This effect has also been reported in macroporous silicon PhCs for statistical deviations of the period due to fabrication tolerances [24].

To explore the limits of the widening strategies, in figure 8(a) structure with 4 groups, 40 modulations and a 100 nm period step has been simulated. It has been compared with two chirped modulations with periods ranging from 1200 nm and 1300 nm to 900 nm in 40 steps. In the four groups case it can be observed that if there is a sufficient number of total modulations, and the 100 nm period step is conserved, the bandgap can be importantly widened. The bandgap width of the four groups' structure is approximately 1850 nm and it can be compared with a chirped PhC with periods from 1300 nm to 900 nm, which presents a very similar bandgap. Thus, as expected from previous results, a wide bandgap in a chirped structure requires more space than the alternatives with periodicity groups. It is reconfirmed that the widest bandgap is obtained with the lower possible number of periodicity groups, always taking into account the overlapping limit. Furthermore, the working wavelength range in the chirped structures is slightly shifted towards the undesired region of longer wavelengths.

PhC with embedded defect

Wide stop-band filters have been theoretically obtained by using structures with multiple periods. In this section, a multiperiodic group structure with a defect has been studied to analyse the possibility of introducing a resonant cavity in the transmission spectrum of a wide bandgap structure to create a narrow passband filter. The structure which offers the widest bandgap with the minimum size in figure 7(a), the PhC with four groups, has been simulated with an embedded resonant cavity. This cavity is basically a straight cylindrical modulation with

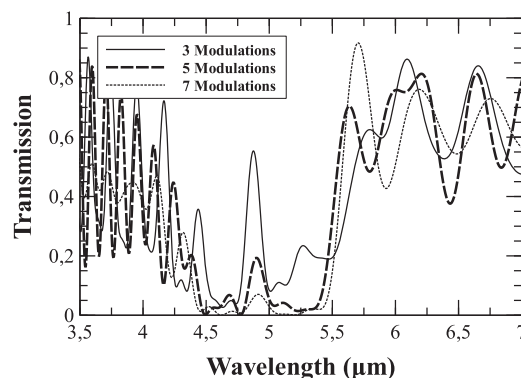


Figure 9. Transmission spectrum of a four group PhC with resonant cavity. The period of the groups is 1050 nm, 1000 nm, 950 nm and 900 nm. The number of modulations has been varied from 3 to 7.

a length of $1.2 \mu\text{m}$ and a diameter of 230 nm—see figure 5. The number of modulations per group has been varied from 3 to 7.

Figure 9 shows the strong dependence of the peak transmission with respect to the number of modulations in the PhC. The approximately exponential decay of the electric field in the PhC causes a fast drop in the peak transmission when longer structures are simulated. It is more difficult for light to couple in and out of the resonant cavity. In the studied case, when 3 modulations per group are simulated the transmission at the resonance peak is around 55.30% and it rapidly decreases to 19.31% for 5 modulations and to 7.04% for 7 modulations. By contrast, the Q factor, calculated as the central wavelength of the peak divided by the difference of wavelength at -3 dB the amplitude of the peak, is kept almost constant when increasing the number of modulations—52, 50, 45 for 3, 5 and 7 modulations per group, respectively—.

From these results, we can conclude that the structure with 5 modulations is the most suitable option for gas spectroscopic sensing. On the one hand, this structure guarantees a wide bandwidth—around $1 \mu\text{m}$. On the other hand, the peak transmission allows the detection of gases. This assertion is based on previous studies where it was found that in a macroporous silicon PhC structure with 18 modulations—similarly to the 20 modulations that we have—the peak amplitude diminished a 20% in a full CO_2 atmosphere [5].

Conclusions

Different alternatives based on multiperiodic modulations have been investigated for an effective widening of the transmission bandgap of macroporous silicon 3D PhCs. It has been shown that by using multiperiodic PhC structures—combining their bandgaps—, the bandgap of macroporous silicon PhCs can be successfully widened and, at the same time, its transmission can be drastically reduced. The reduction of the transmission in the bandgap is mainly explained by the addition of modulations to the PhC, which drastically decreases the offset while maintains a similar transmission amplitude outside the bandgap. The number of modulations also determines the slope of the bandgap edges. The bandgap widening is due to the successful concatenation of the individual bandgaps of the periodicity groups or modulations—in the chirped case—.

Bandgaps of approximately $1 \mu\text{m}$ and $1.8 \mu\text{m}$ have been obtained with four periodicity groups and chirped structures. However, even though all the alternatives are valid for bandgap widening, the suitability of each bandgap widening alternative depends on the desired spectral bandgap response. Thus, a certain possibility of engineering the bandgap is introduced. The structure which offers the widest bandgap with the shortest length is the one with the minimum possible periodicity groups, in this case defined by the 100 nm maximum period difference. If smoother responses—inside and outside the bandgap—or higher tolerance to fabrication period deviations are desired, the chirped alternative is the best choice. Furthermore, the slope of the bandgap edges can be steeper by adding more modulations while maintaining constant the periodicity.

Finally, it has been observed that a resonant peak, whose Q-factor is almost independent of the PhC's length, can be introduced in the $1 \mu\text{m}$ wide bandgap of a multiperiodic PhC by means of a resonant cavity defect. The results have revealed that a trade-off exists between the length of the PhC and the transmission of the resonant peak. On the one hand, long PhCs—with a significant number of modulations per group—allow smooth bandgaps with almost null transmission, however, the obtained resonant peak has low transmission because of the low light injection into the cavity. On the other hand, short PhCs result in resonant peaks with high transmission but the resulting bandgaps are smaller and present meaningful transmission. For spectroscopic gas

sensing, an optimal structure with 4 periodicity groups with 5 modulations each is proposed. Placing defects in structures with wider bandgaps would require mechanisms to pump light into the central defect.

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