Thermal emission properties of 2D and 3D silicon photonic crystals

Benjamin Gesemann a,*, Stefan L. Schweizer a, Ralf B. Wehrspohn a,b

a Institute of Physics, Martin Luther University Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle, Germany
b Fraunhofer Institute for Mechanics of Materials, Walter-Hülse-Str. 1, 06120 Halle, Germany

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Abstract

We present measurements of the thermal emission properties of 2D and 3D silicon photonic crystals with and without substrate heated resistively as well as passively with an aluminium hotplate. The out-of-plane and in-plane emission properties were recorded and compared to numerical simulation. It turned out that for the in-plane 2D photonic crystal and out-of-plane 3D photonic crystal emission a photonic stop gap effect is visible. For the out-of-plane 2D photonic crystal emission, no photonic bandgap effect is observable but instead strong silicon oxide emission from native oxide inside the pores of silicon are observable. A model for the modified thermal emission is presented.

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1. Introduction

In the last decade the fabrication and the optical properties of photonic crystals have been extensively studied. In particular, two dimensional (2D) photonic crystals provide a wide range of applications due to their good compatibility with classical integrated optics and rather simple fabrication processes compared to 3D photonic crystals. Although there are lots of publications on monochromatic beam propagation issues and subsequent applications like microresonators, filters, waveguides etc. only few experimental measurements of broadband emission/coupling features at the crystal–air interface can be found [1–3]. Recently, photonic crystals have been suggested for ultra-compact sensors [4] as well as for selective thermal emitters. Based on the photonic bandstructure, the photonic density of states (DOS) inside the 2D or 3D photonic crystal provides some interesting regions like slow modes near the band-edges or no states inside the gap-regions which could be usefull to control the thermal radiation. First experimental realizations of spectrally selective thermal emitters have been carried out by either using 2D metallic grating couplers on 2D photonic crystals [5] or 3D metallic woodpiles stacks [6]. From a thermodynamical point of view, the selective thermal emission will not be stronger than that of a black body [7]. However, due to the lower integrated spectral emissivity, a lower power consumption is expected compared to a black body which is advantageous for mobile, energy-saving sensing application.

We report on the spectral modification of the thermal emission of 2D and 3D silicon photonic crystals compared to bulk material by heating the photonic...
crystal directly by DC currents and passively with external hotplates.

2. Experimental

2D and 3D silicon photonic crystals were fabricated by photo-electrochemical etching using prepatterned n-type silicon wafers [8,9]. The lattice constant of the photonic crystals was \( a = 2 \ \mu m \) and \( a = 4.2 \ \mu m \) and pore radius was nominal 800 nm/1.7 \( \mu m \) (100%). We used n-type silicon wafers with a thickness of 500 \( \mu m \). The depth of the pores was 400 \( \mu m \) in the case of 2D and 3D. To create membranes, the resisting 100 \( \mu m \) of bulk silicon has been released electrochemically. The lattice constant and in-plane geometry of the crystals have been determined by photolithography (Fig. 1).

Sample emission spectroscopy was carried out using a Fourier-transform infrared spectrometer (FTIR) Bruker IFS 66 with an additional channel for external light source characterization. For initial measurements (Section 3.1) the light was directly focused on the probe-spot without additional IR-optics so that a resolution of approximately 1.4 mm FWHM at the probe surface was achieved. The numerical apertur of the detection unit was \( NA \approx 0.14 \). Surface emission has been measured at different heating currents normal to the 4.0 mm \( \times 4.7 \) mm probe surface. As reference, a similarly sized bulk-silicon sample was taken. Since the absolute sample temperature could not be measured, the emissivities of the photonic crystals were compared always to non-structured sample emissions at similar detection intensities. For local emission measurements a Hyperion 1000 IR microscope was used in combination with the FTIR Spectrometer and the samples were heated passively by a hotplate. Numerical simulations have been performed using a commercially available finite element code (COMSOL Multiphysics) as well as the free MPB [10] tool for 3D bandstructure calculations.

3. Results

3.1. Out-of-plane emission from 2D and 3D silicon photonic crystals

To measure the thermal emission parallel (out-of-plane) to the photonic crystal pores, the photonic crystal itself was electrical contacted at both sides and heated via DC currents. To verify the influence of the 2D photonic band structure on the out-of-plane emission spectrum, samples with different lattice constants were heated passively by a hotplate. Numerical simulations have been performed using a commercially available finite element code (COMSOL Multiphysics) as well as the free MPB [10] tool for 3D bandstructure calculations.

![Fig. 1. SEM micrograph of a photoelectrochemically etched 2D silicon photonic crystal (lattice constant \( a = 4.2 \ \mu m \)) with vertical etched trench as crystal sideface to separate multiple samples. Thermal emission was measured longitudinal (parallel to the crystal pores) as well as transversal (perpendicular to the pores, normal to the sideface).](image1)

![Fig. 2. Out-of-plane (parallel to the crystal pores) emission measurements of 2D silicon photonic crystals compared to bulk silicon emission at different temperatures. Top: Thermal emission spectra compared to bulk silicon samples for different temperatures. Bottom: Emission spectra for crystals with different lattice constants compared to bulk silicon emission. For comparison, the integrated area below each spectrum is inserted in the diagramm.](image2)
used. Compared to the thermal emission of bulk silicon the measured out of plane emission spectra of a 2D periodically structured samples show a sharp emission peak around 1100 cm$^{-1}$ (Fig. 2A) and suppressed emission at higher frequencies. Whereas the maximum of the emission of a black body shifts with temperatures according to Wien’s displacement law (Fig. 2A), the highly selective emission of the porous sample leads to a fixed peak at common temperatures. By measuring the emission spectra of crystals with different lattice constants, it is verified that the peak emission of the out-of-plane emissivity is not affected by the lattice constant and thus the in-plane photonic band structure (Fig. 2B). The strong selective emission can be explained by the enhanced silicon oxide surface emission of the inner pore sidewalls. The measured peak is in accordance to a vibrational Si–O band[11]. Due to the high silicon oxide ratio caused by the porosity, the oxide emission dominates the emission spectrum. Since the absolute temperature of the samples could not be measured for the dc heated samples, the spectra were taken at equal emission amplitudes around the peak frequency around 1050 cm$^{-1}$ in each case.

By appropriate control of the etching parameters, the pore diameter can be varied during the etching process [12]. In combination with the lithographic hexagonal surface patterning an inverted simple hexagonal (sh) 3D photonic crystal can be fabricated. Note, it is also possible to fabricate simple cubic photonic crystals by using square lithographic patterns [13]. We define the out-of-plane emission direction of the 3D photonic crystals being the $\Gamma$–A direction. However, due to the numerical aperture of the measuring setup also fractions of $\Gamma$–L to $\Gamma$–H emission will be detected. Fig. 3B shows the measured emission spectra of the inverted simple hexagonal 3D photonic crystals. The periodical modulation of the pore diameter results in a narrow dip in the emission spectrum according to a stop gap in the $\Gamma$–A direction shown in Fig. 3A. By changing the modulation length and thus the lattice constant in $\Gamma$–A direction, the position of the dip can be linearly shifted with only marginal influence on the lower bands in the $\Gamma$–M–K plane. Our results for the emission dip for modulations along the pore axis are in agreement with [14]. In contrast to the 2D membranes, we could not observe the same selective oxide peak for samples with modulated pores on resisting bulk silicon. For a correct interpretation of the differences in the emission spectra, some details about the used materials and thermal emission mechanisms have to be taken into account. The photoelectrochemical etching process requires a thin highly doped layer on the backside. Hence the backside acts like a high emissivity broadband emitter that covers potentially selective emission from over-lying crystal structures. Due to thermodynamically consistent absorption and re-emission mechanisms, selective emission features of overlying layers were covered by the backside emission.

To verify the influence of the backside emission on the measured spectra, we compared 2D photonic crystal spectra with and without (membranes) substrate. Fig. 4 shows the resulting spectra. As predicted, samples with remaining substrate show a broadband blackbody like emissivity with just the characteristic atmospheric absorptions like CO$_2$ and H$_2$O, whereas membranes show a pronounced Si–O bond peak around 1100 cm$^{-1}$. In contrast to prior emission measurements with direct DC heated samples and whithout microscope coupling, we observed a double peak around 2200 cm$^{-1}$ next to the CO$_2$ dip. Structures with different lattice constants (2 $\mu$m and 4.2 $\mu$m) were used to verify if this spectral feature is based upon photonic crystal effects. There is

Fig. 3. Left: SEM image of a 3D silicon photonic crystal. Cut along the pore axes. They were fabricated by modulating the 2D photonic crystals pore diameters along the pore axis during the etching process. Center: Calculated band structure for photonic crystals with same in-plane lattice constant $a=2$ $\mu$m in the $\Gamma$–M–K plane but different lattice constants $d$ in $\Gamma$–A direction. Right: Emission spectra for two different lattice constants $d$ in $\Gamma$–A direction compared to a non-modulated hexagonal 2D photonic crystal. The corresponding frequency regions for the $\Gamma$–A stop gaps were marked in dark grey (region I) for $d=3$ $\mu$m and light gray (region II) for $d=2$ $\mu$m.
no correlation between the photonic bandstructure and the measured peaks because the peak positions were stable for different lattice constants. We suppose contaminations for example by dopants or the aluminium hotplate to be responsible for the emission at 2100 cm\(^{-1}\) and 2260 cm\(^{-1}\).

### 3.2. In-plane emission from the 2D silicon photonic crystal sideface

By using an IR microscope to couple the probe emission into the FTIR spectrometer we were able to decrease the spotsizes down to several tens of microns (with additional apertures). The exact position of the spot can be controlled in the visible range. This enables us to collect thermal emission from the photonic crystals sideface perpendicular to the crystal pores. Fig. 5 shows the measured emissivities of two different samples with lattice constants of of \(a = 2 \, \mu m\) (black curve) and \(a = 4.2 \, \mu m\) (red curve). In accordance to the emissivity measurements of 3D structures (Section 3.1) and the simulated 2D bandstructure (Fig. 5), the out-of-plane measurements also show decreased emissivities at bandgap frequencies between 600 cm\(^{-1}\) and 950 cm\(^{-1}\) for the 4.2 \(\mu m\) structures and respectively 1250 cm\(^{-1}\) to 2000 cm\(^{-1}\) for the 2 \(\mu m\) structures. The upper band edge for the 2 \(\mu m\) structure at 2000 cm\(^{-1}\) is not as strong visible as the 950 cm\(^{-1}\) band edge due to the materials low absolute emissivity in this frequency region.

### 4. Discussion

When measuring the emissivity in direction of a bandgap, either out-of-plane emission from 3D photonic crystals or in-plane emission out of 2D photonic crystals, we observed decreased emissivity within bandgap frequencies. This is however only possible when there is a temperature gradient on the sample as expected from our measurement setup. If the whole crystal would be on exactly the same temperature, there would be not filter effect due to equilibrium of absorption and reemission. Only a grating effect (diffraction) of the external photonic crystal patterning would be observable. This assumption is supported by the out-of-plane measurements on 2D photonic crystals where no bandgap effect is present. Instead we observe an strong emission of the silicon-oxide covering the pore walls. The photonic crystal just acts like a filter for thermal emission.

### 5. Conclusion

We carried out a detailed study to understand the thermal emission properties of 2D and 3D silicon...
photonic crystals. It turned out that we do not see any features of the 2D in-plane bandstructure in the out-of-plane emission spectrum of pure 2D photonic crystals. However an enhanced emission peak of the thermal silicon oxide could be observed and explained by the highly porous structures.

By introducing an additional periodicity in the out-of-plane direction we produced 3D photonic crystals that may act as tunable thermal emitters with large emitting surfaces. Regarding the influence of the stop-gap our results are in agreement with Garín et al. [14]. We extended the theory of the photonic crystal emission and discussed the influence of the substrate-layer that significantly affects the emission characteristics. We also extended the measurements to in-plane emission measurements of 2D photonic crystals where we observed suppressed emissivity within bandgap frequencies in accordance to the 3D crystal surface measurements.

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References
