Periodically arranged point defects in two-dimensional photonic crystals

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We present and characterize point defects in a two-dimensional photonic crystal based on macroporous silicon. These point defects are prepatterned periodically, forming a superlattice within the photonic crystal. Spatially resolved optical investigations, related to morphological properties such as defect concentration and pore radius, are compared to ab initio band-structure calculations. The spatially confined defect states are identified and their interaction is evaluated quantitatively by applying a tight-binding model to describe the formation of bands.

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Photonic bandgap materials have extensively been studied in recent years.1 By applying theoretical methods of solid state physics to periodic dielectric structures, the prediction of their properties and behavior has become possible.2 Structures disturbing the periodicity of the photonic crystal are of special interest, because they may act as confining or guiding elements for light. If, for instance, a point defect is introduced, defect levels within the photonic bandgap will arise. Their behavior can be donor-like or acceptor-like, according to the type of the perturbation.3 Strictly speaking, a single point defect breaks the translational symmetry of the crystal and a band structure, based on the Bloch-Floquet theorem, no longer exists.

A first theoretical approach describing interacting resonators was proposed by Yariv et al.4 The coupled-resonator optical waveguide relies on evanescent field coupling of resonator modes of adjacent resonators. Similar structures were realized by a linear arrangement of point defects in photonic crystals.4,5 A formation of bands within the photonic bandgap was observed. However, breaking of the two-dimensional (2D) symmetry allows the presentation only in a one-dimensional projected band structure. Possible applications of these structures are, e.g., dispersion compensators,6 coupled cavity lasers,7 and delay components in optical circuits.8

In this communication, a periodic arrangement of point defects is studied theoretically and experimentally. This is somehow similar to the doping of semiconductors, whereby a dopant is distributed statistically at preferred sites of the atomic lattice. A successive increase of the defect concentration allows the investigation of the point defect interactions. Furthermore, a band structure for the superstructure within the 2D photonic crystal has been calculated applying either plane wave approaches or tight-binding analysis.

Macroporous silicon is a very suitable model system for photonic crystals. The high refractive index contrast allows the fabrication of structures with complete photonic bandgaps. 2D photonic crystals in the near infrared have been already fabricated and studied.9–11 The 2D photonic crystals consist of highly ordered macropores prepared by an electrochemical etching process.12,13 The pores are etched in hydrofluoric acid by applying a photoelectrochemical dissolution process. Using lithographic prestructuring, the nucleation sites of the pores can be defined at the surface of the n-type silicon wafer. This allows one to control pore pattern and lattice constant (unit a). During the etching process, the backside of the wafer must be illuminated to generate electronic holes in the silicon, which are consumed by the dissolution of silicon. Due to electrochemical passivation of the pore walls, very high aspect ratios (length/diameter) of 100–500 can be obtained. Therefore, macroporous silicon represents an excellent system to study 2D photonic crystal properties.

The lithographic prestructuring before the etching process allows setting and also omitting single pores in the hexagonal lattice of the photonic crystal as well as the creation of superperiodicity. The investigated structure is a hexagonal cavity similar to H2 cavities, reported by Olivier et al.5 An H2 cavity is a point defect in a hexagonal 2D photonic crystal and consists of seven missing pores. In contrast to the H2 structure, in our structures a central pore is introduced to create a hexagonal ring, shown in Fig. 1(a). The lattice constant of the host crystal is 700 nm.

This point defect geometry causes two types of disturbances. The six missing pores in the hexagonal ring introduce more dielectric material into the crystal. Furthermore, the pores around the defect as well as the center pore show slightly larger diameters than all the other pores of the crystal. This is caused by the so-called proximity effect. During the etching process, the electronic holes that are not consumed by a missing pore are consumed by the surrounding pores, leading to larger diameters.

The defects studied here are arranged in a hexagonal lattice according to the symmetry of the photonic crystal. This can be revealed by a Fourier transformation of scanning electron microscope (SEM) images, as shown in Fig. 1(b). In between each of the six spots of the perfect photonic crystal and the center (distance a*) a hexagonal pattern appears with distances a*/d, where d·a is the distance between two defects in real space. Experimentally, this can be visualized by laser surface diffraction. A parallel laser beam is directed onto the surface of the crystal parallel to the pores. The directly reflected intensity is detected on a flat screen and registered by a digital camera. If the wavelength of the laser...
The fully vectorial algorithm calculates the frequency eigenstates of Maxwell’s equations.14,15 The different pore diameters caused by the proximity effect. Iterative eigenstates and the electromagnetic field modes. A change of the defect concentration is achievable by a variation of the distance between the hexagonal rings. As shown in Figs. 2(a)–2(c), the distance between the defects varies from 6 to 13 lattice constants in Γ-K direction. In principle, any integer value larger 3 of the lattice constant can be chosen. The corresponding defect concentrations are between 8.73 × 10^4 cm^-2 and 1.86 × 10^4 cm^-2.

For a theoretical study of the electromagnetic properties of the photonic crystal, a frequency-domain-based method is used, with the model of the point defect superstructure coded on a 2D supercell grid. This allows us to take into account the different pore diameters caused by the proximity effect. The fully vectorial algorithm calculates the frequency eigenstates and the electromagnetic field modes. Iterative eigensolvers are applied to find an adjustable number of the lowest eigenstates of Maxwell’s equations.14,15

For an experimental characterization of the photonic crystal structures, optical investigations are essential. Therefore, Fourier transform infrared (FTIR) reflection measurements were performed by coupling light perpendicularly into the cleaved facet of the pores of the 2D photonic crystal and detecting the specular reflected light in the plane of periodicity using an IR microscope (numerical aperture 0.4) coupled to the FTIR spectrometer.

For the unperturbed crystal, the reflection spectrum in Γ-M direction exhibits a broad frequency range (from 0.22 to 0.34 norm. frequency, TE-polarization) of high reflectivity (Fig. 3). Comparing this spectrum to the corresponding band structure, the region of high reflectivity and fundamental bandgap match well. Light of frequencies in the bandgap cannot enter the crystal and will be reflected by interference total reflection. Furthermore, higher bands can be probed by comparing the features of the reflection spectrum with respect to the band symmetry between the high symmetry points.16 Since a plane wave in free space has a constant phase perpendicular to the propagation direction, coupling bands have to fulfill certain symmetry properties regarding this propagation direction. Therefore, noncoupling bands are displayed as dashed lines in Fig. 3. A similar reflection spectrum can also be obtained for the Γ-K direction. Small deviations in the spectral position can be attributed to a slightly nonspherical shape of the pores of the real structures. This causes a symmetry reduction and therefore a small shift in the band structure.17 The fact that the reflectivity does not reach unity is related to the acceptance angle of the microscope objective. Light that does not hit the cleaved facet perfectly perpendicularly can be reflected nonspecularly and it is therefore not detected by the objective again. Furthermore, the termination of the facet also plays an important role and may cause nonspecular reflection.18

A reflection spectrum for a crystal including point defects (defect concentration 1.86 × 10^4 cm^-2) is shown in Fig. 4(a). The plateau of high reflectivity shows several notches of lower reflectivity. By comparing the reflection measurement to the corresponding band structure, these notches are clearly identified as defect states within the photonic bandgap. The correspondence of the reflectivity spectrum to the bandstructure calculation (Fig. 4) is slightly inferior to that of the bulk photonic crystal (Fig. 3), since the nonsperical shape of the pores has a significantly higher influence on the spectral position of the resonator modes. For frequencies of the photonic bandgap, the wave has a certain penetration depth and therefore a coupling to resonators within this depth is possible. The plane wave \( E = E_0 e^{i(k_x x + k_y y - \omega t)} \) couples to a defect state via evanescent field coupling if the frequency \( \omega_0 \) is resonant to the defect state. This can be described by a complex wave vector \( \mathbf{k} = k_x + ik_y \), with \( k_y \gg k_x \). This incoming plane wave will then be transformed to a resonator mode. Impedance mismatch of the incoming wave and the resonator modes does not occur.13

![Image](image_url)
The band structure shows 18 states within the first photonic bandgap for TE polarization [Fig. 4(a)]. These states are energetically separated and form discrete levels within the bandgap. This is a clear indication for separated point defects within the crystal. Due to their distance of 13 lattice constants, they are hardly interacting.

The large number of defect levels can be explained by the complex defect geometry. Two types of defect states are expected, dielectric defects caused by the six missing pores and air defects caused by larger pores during the etching process (proximity effect). A detailed group theoretical classification according to Sakoda\textsuperscript{16} shows that the external plane wave only couples to those resonator modes that fulfill the required symmetry conditions. For the $\Gamma$-$M$ direction shown here, the number of modes that couple to a plane wave reduces from 18 to 10. Increasing the defect concentration to $4.91 \times 10^4 \text{ cm}^{-2}$ (corresponding to a defect distance of 8 lattice constants) causes even more pronounced notches in the high reflectivity region [Fig. 4(b)]. Light entering the crystal couples to more resonators close to the surface of the cleaved pores. The number of the coupling resonators is proportional to the defect density and should therefore scale linearly with the reflectivity. Since the discrete levels of the band structure indicate hardly interacting resonators, light once having entered the resonator will be lost by scattering out of the plane of periodicity or by coupling to the silicon substrate.\textsuperscript{19}

After a further increase of the defect concentration ($1.26 \times 10^5 \text{ cm}^{-2}$, distance of 5 lattice constants) only several peaks of high reflectivity remain in the spectrum [Fig. 4(c)]. The reason for these peaks is the overlapping of defect modes. This is shown via the corresponding band structure (Fig. 4); discrete levels begin to form bands within the bandgap. A bending of levels towards the air and dielectric bands, respectively, takes place. Only small gaps remain in between bands of defect levels [Fig. 4(c)]. In contrast to the lower defect concentrations, the complete band structure of the superstructure is plotted (red).

To extrapolate this behavior, a band structure for a defect density of $1.96 \times 10^5 \text{ cm}^{-2}$ (defect distance of 4 lattice constants) is calculated [Fig. 4(d)]. Within the host bandgap, several groups of bands are formed. Smaller gaps remain in between them. The host bandgap splits up into two smaller gaps.

The formation of bands due to overlapping resonator modes can be visualized by a periodic continuation of the field distribution in the supercell, displayed in Fig. 5. For a defect concentration of $4.91 \times 10^4 \text{ cm}^{-2}$ [Fig. 5(a)] the field is well localized around the resonator, whereas for a defect concentration of $1.26 \times 10^5 \text{ cm}^{-2}$ the field distributions of adjacent resonators begin to overlap and the resonators therefore interact [Fig. 5(b)].

To characterize the interaction of the resonators quantitatively, a tight-binding model, as proposed in Refs. 3 and 20, can be applied. Since the resonator modes are well localized and show a weak angular dependence, it is possible to describe the dispersion relation of these bands by

$$\omega_{\text{resonant}}(\mathbf{k}) = A + \frac{B}{2} \sum_{n.n.} \cos(\mathbf{k}d).$$

Parameter $A$ corresponds to the average frequency of the band, parameter $B$ is the bandwidth. The summation runs over the next neighbors (n.n.). A fit of this model to a calculated resonator band within the irreducible Brillouin zone is displayed in Fig. 5(c). Since $B$ is clearly a measure for the

FIG. 3. Reflection measurement of a 2D photonic crystal without point defects (lattice constant 700 nm, TE polarization) compared to the corresponding band structure ($r/a$=0.36); dashed: noncoupling bands.

FIG. 4. (a) Reflection measurement ($\Gamma$-$M$ direction, $r/a$=0.36, TE polarization) of a photonic crystal containing point defects (defect concentration $1.86 \times 10^3 \text{ cm}^{-2}$, distance 13 lattice constants) compared to a band-structure calculation (defect levels-red, bands of the host crystal-black); (b) same as (a) but for a defect concentration of $4.91 \times 10^4 \text{ cm}^{-2}$, distance 8 lattice constants; (c) same as (a) but for a defect concentration of $1.26 \times 10^5 \text{ cm}^{-2}$, distance 5 lattice constants; and (d) band structure for a defect concentration of $1.96 \times 10^5 \text{ cm}^{-2}$, distance 4 lattice constants.
interaction of the resonators, it is averaged for all defect levels within the photonic bandgap and plotted versus the defect distance for the $\Gamma$-$M$ direction and $\Gamma$-$K$ direction. Figure 5(d) shows an exponential decay of $B$ with the defect distance $D$, which can be described by $B \propto e^{-D/\gamma}$. The decay constant $\gamma$ has been estimated to be 0.81 $a$ and 0.82 $a$ for the $\Gamma$-$M$ direction and the $\Gamma$-$K$ direction, respectively.

In conclusion, this article describes a superstructure of resonators in a 2D photonic crystal. The comparison of the optical properties, investigated by reflection measurements and band-structure calculations, shows a formation of bands from discrete defect levels with decreasing defect distance. This is caused by an interaction of adjacent point defects due to their overlapping resonator modes. A tight-binding model can be applied to characterize the interaction quantitatively.

The introduction of periodic point defects to a photonic crystal lattice opens a way to tailor the band structure with respect to the group velocity or the dispersion. Such low-group-velocity structures could be potentially applied as delay components in optical circuits or as size-reducing elements in dispersion compensators.

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