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Effect of Disorder on the Electromagnetic Properties of Photonic Crystals

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Real photonic crystals suffer from imperfections due to inaccuracies in manufacture. Therefore these imperfections have to be taken into account as disorder in the lattice structure when the properties of photonic crystals are simulated. Here, in particular the effect of positional and radial disorder on the density-of-states and on the mode structure of electromagnetic waves in a photonic crystal is studied for 2D systems.

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1. Introduction

Photonic crystals (PhCs) are structures with a (nominally) exactly periodic variation of the dielectric constant or the permeability. There is a similarity between the laws governing the propagation of electromagnetic waves in a PhC and the laws for the motion of electrons in the periodic potential of a lattice of atoms. In both cases the Bloch theorem holds and the wave function can be described as a Bloch function: the product of a lattice periodic function $u_{nk}(\boldsymbol{r})$ and a slowler varying oscillatory function $\exp(\mathrm{i}\boldsymbol{kr})$.

When PhCs are manufactured, e.g. by etching a two-dimensional array of cylindrical holes into a semiconductor, deviations from the ideal periodicity can occur [1]. The positions of the axes of the cylinders will deviate from the lattice positions (positional disorder). The radii of the cross-sections of the cylinders will vary, e.g., due to slight variations in the etching rate (radial or size disorder). Taking into account the three-dimensionality of the structure, positional and radial disorder may occur also along each hole. The cross-section of the hole, e.g., may decrease with increasing distance from the semiconductor surface. Similar variations occur for arrays of free-standing rods produced by etching. For self-assembled structures, stacking faults [2] or the occurrence of a polycrystalline grain structure [3] are further possible sources of disorder.

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In this work we study 2D PhCs and concentrate on positional and size disorder on two-dimensional arrays of rods (dielectric constant higher than in the background). Such an array has been used [4, 5] to investigate negative refraction.

2. Modelling the disorder

In this work as a starting point a two-dimensional array of rods arranged on a square lattice (see left diagram of Fig. 1) is chosen. The ratio of rod radius r to lattice constant a is chosen to be $r/a = 0.329$. A dielectric constant of $\epsilon = 13$ is assumed for rods of the square lattice. The rods are surrounded by air ($\epsilon = 1$). The band structure of this system is shown in Fig. 2.

The positional disorder of a 2D PhC can be described as a random shift $(\delta_{x,i}, \delta_{y,i})$ of each rod (index i see moddle diagram of Fig. 1). This shift is limited by the parameter δ_{p}, $\delta_{x,i} < \delta_{\mathrm{p}}$, $\delta_{y,i} < \delta_{\mathrm{p}}$. The random values $\delta_{x,i}$ and $\delta_{y,i}$ are

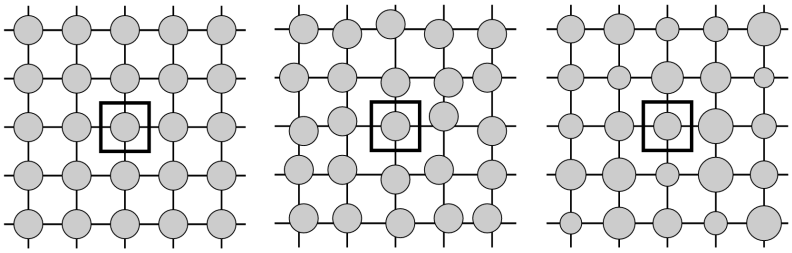

Fig. 1. Positional and size disorder: left — perfect crystal, middle — crystal subject to positional disorder, right — size disorder. The intersections of the lines indicate the centers of the rods in the perfect crystal. The square indicates the unit cell of the perfect PhC.

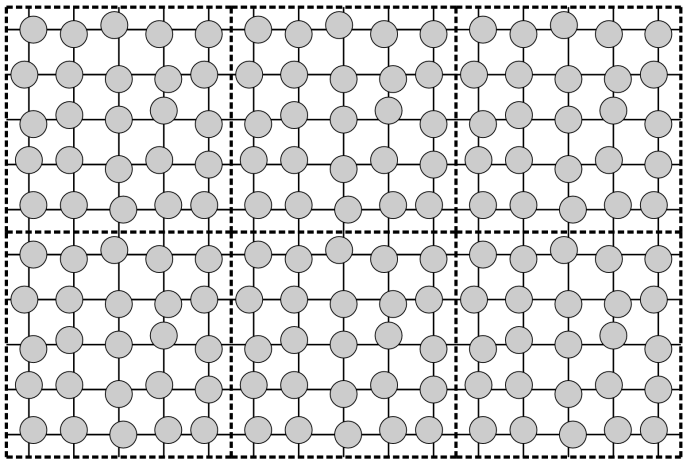

Fig. 2. Band structure for a perfect ($\delta_{\mathrm{p}} = \delta_{\mathrm{r}} = 0$) square lattice of rods. $r/a = 0.329$, $\epsilon = 13$ (TM polarization). After Ref. [6].

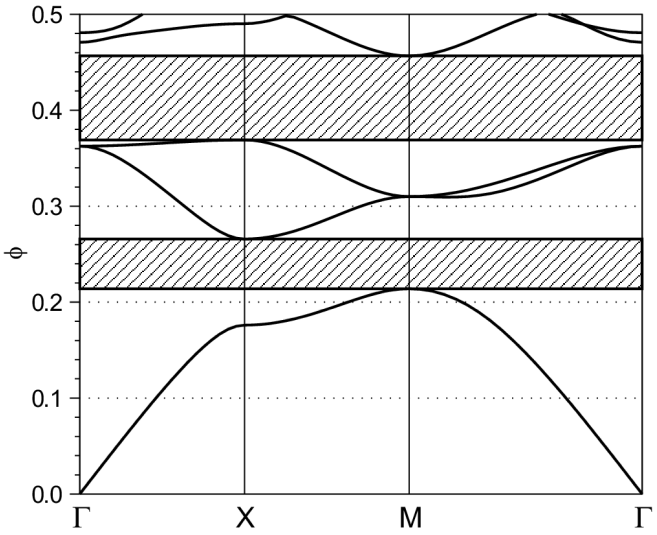

Fig. 3. Crystal constructed from disordered supercells. The dashed lines indicate the boundaries of the repeated supercells.

uniformly distributed. In this way δ_{p} controls the amount of disorder — for $\delta_{\mathrm{p}} = 0$ the PhC is perfectly ordered. Radial disorder is described in a similar way as a variation of the radius of the i-th rod $r_i = r + \delta_{\mathrm{r},i}$, with $\delta_{\mathrm{r},i} < \delta_{\mathrm{r}}$ (see righr diagram of Fig. 1).

For an (ideal) PhC a number of mathematical methods are available. The band structure of the PhC can be calculated, e.g., using the plane wave expansion (PWE) method [7]. Strictly speaking, in the presence of disorder, the Bloch theorem is no longer valid. However, in order to be still able to employ the methods an approximation of the disordered crystal has to be used. This is done by extracting a supercell [8] consisting of N rows and N columns of unit cells from the disordered crystal and using this supercell as the new unit cell for a PhC (see Fig. 3). As the area of the unit cell in real space is increased by a factor of N^2 the area of the corresponding Brillouin zone decreases by N^{-2}. The band structure is then calculated for this PhC for N_k different wave vectors. To avoid artefacts, e.g. by choosing symmetrical points, these wave vectors are chosen at random from positions in the supercell Brillouin zone.

To determine the density-of-states the frequency region of interest is divided into intervals of equal width. Then, for each interval the number of eigenstates with frequencies in this interval is counted, determining the denstty-of-states up to a constant factor, i.e. in arbitrary units (a.u.). As shown in Fig. 4 increasing the number of wave vectors beyond $N_k = 50$ does not increase the precision in the determination of the density of states significantly. Calculation times increase very fast with increasing N. Therefore, $N = 10$ and $N_k = 50$ were chosen for the determination of the density-of-states.

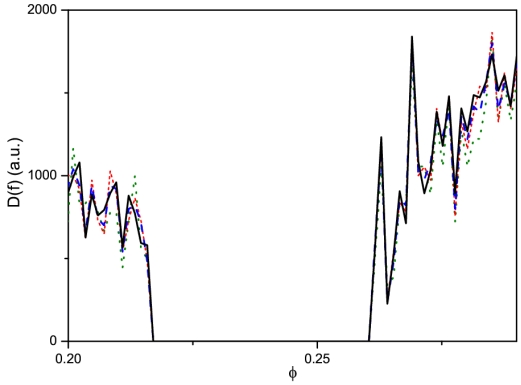

Fig. 4. Comparison of the calculated density-of-states using different values of N_k (the number of wave vectors) for a 10×10 supercell and TM polarization, (solid — $N_k = 150$, dashed — $N_k = 50$, short dashed — $N_k = 37$, dotted — $N_k = 18$). Positional disorder $\delta = 0.1a$, TM polarization.

The states of the electromagnetic wave in a PhC scale with the lattice constant a. If a is increased by some factor κ the corresponding states in the magnified PhC have frequencies reduced by a factor of $1/\kappa$. Therefore results will be given in terms of the reduced frequency $\phi = fa/c$ and can be scaled to the lattice constant chosen.

3. Results and discussion

3.1. Density-of-states

The effect of positional disorder on the density-of-states is shown in Fig. 5, the effect of radial disorder is shown in Fig. 6. In both cases as the degree of disorder is increased the width of the gap is narrowed. The second gap is more sensitive to disorder and shows this narrowing effect earlier. This may be explained by the shorter wave length of the electromagnetic waves in the air and in the rods for frequencies in the second gap than in the first gap. Therefore, at higher frequencies, the sensitivity to variations in the spatial dimensions is increased. This is true also for the higher bands, but is more conspicuous for the second gap.

As the disorder is increased, not only is the gap narrowed, but also states within the gap appear. Again the second gap is more sensitive to disorder.

Qualitatively, this happens both for positional and radial disorder. However, smaller values of the radial disorder parameter δ_{r} compared to the corresponding values of δ_{p} for positional disorder are sufficient for these effects. This difference is more pronounced for stronger disorder.

3.2. Modes structure

To study the effect of positional and radial disorder, respectively, in more detail, the electromagnetic modes, the eigenstates of the electromagnetic field in the supercell PhC are examined. Since less states have to be determined from

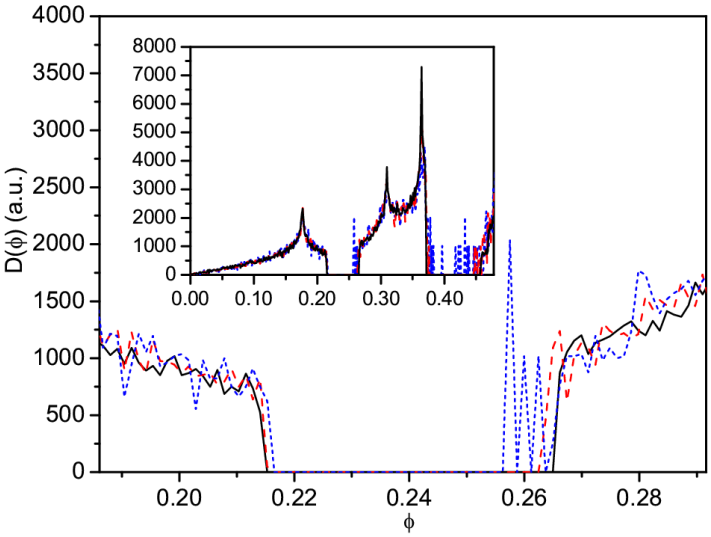

Fig. 5. Density-of-states vs. reduced frequency $\phi = fa/c$ for the square lattice of rods for the TM polarisation in the region around the first gap (inset: full plot up to the edge of the third band) for *positional* disorder. Bold — no disorder, dashed — $\delta_{\mathrm{p}} = 0.05a$, short dashed curve — $\delta_{\mathrm{p}} = 0.1a$.

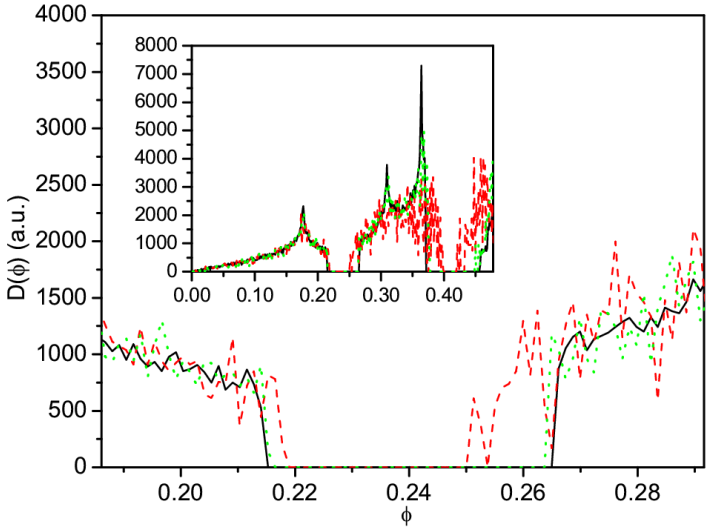

Fig. 6. Density-of-states vs. reduced frequency $\phi = fa/c$ for the square lattice of rods for the TM polarisation for the region around the first gap (inset — full plot up to the edge of the third band) for *radial* disorder. Solid curve — no disorder. Dotted curve — $\delta_{\mathrm{r}} = 0.02a$. Dashed curve — $\delta_{\mathrm{r}} = 0.05a$.

the calculation it is feasible to increase the size of the supercell in this case to 20×20. For modes with frequencies in a band of the photonic band structure a direct comparison with the mode closest in frequency of the supercell with $\delta_{\mathrm{p}} = 0$ and $\delta_{\mathrm{r}} = 0$ is possible. For positional disorder ($\delta_{\mathrm{p}} = 0.1a$) and a reduced frequency of $\phi = 0.212$ this is the mode shown in Fig. 7 in the top-right diagram, for radial disorder ($\delta_{\mathrm{r}} = 0.05a$) the mode is shown in the left diagram of Fig. 8. The corresponding mode in the absence of disorder is shown at the top left in Fig. 7. As a consequence of frequency degeneracy this mode appears as a diamond pattern due to a superposition of two Bloch waves. This pattern, although deformed, is also seen in the mode of the PhC with positional disorder — the degeneracy is not broken by the random disorder. In the case of radial disorder the pattern is even stronger deformed and weakly recognizable.

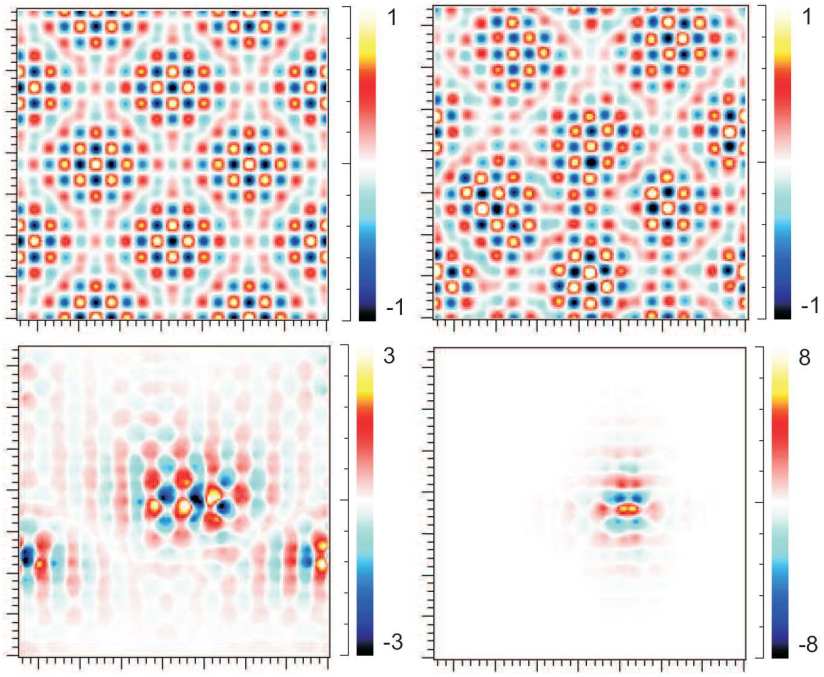

Fig. 7. Distribution of the electrical field for TM polarized electromagnetic eigenstates in the perfect PhC and in a PhC with *positional* disorder $\delta_{\mathrm{p}} = 0.1a$. Top left diagram: mode of the perfect $\delta_{\mathrm{p}} = 0$ PhC for a frequency in the lowest band. The reduced frequency is $\phi = fa/c = 0.212$. Modes of electromagnetic eigenstates in the disordered ($\delta_{\mathrm{p}} = 0.1a$) PhC. Top right diagram: $\phi = 0.212$ (as for top left). Bottom left diagram: $\phi = 0.264$, i.e., at the lower edge of the second band (in the frequency region of the first gap of the perfect PhC). Bottom right diagram: $\phi = 0.253$, in first band gap near the second band. After Ref. [6].

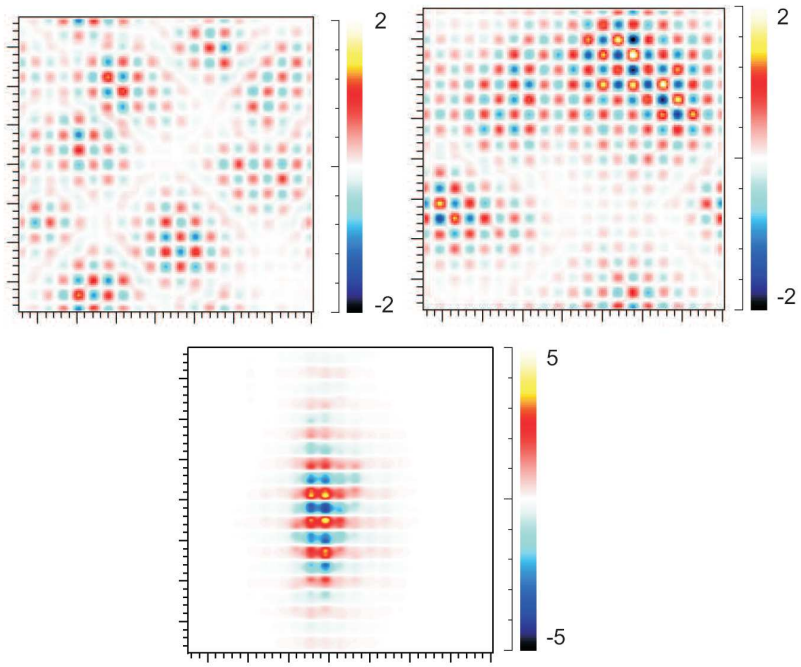

Fig. 8. Distribution of the electrical field for TM polarized electromagnetic eigenstates in a PhC with *radial* disorder $\delta_r = 0.05a$. Top left diagram — $\phi = 0.212$, in the lowest band. Top left diagram — $\phi = 0.216$, at the upper edge of the lowest band (in the frequency region of the first gap of the perfect PhC). Bottom diagram — $\phi = 0.251$, in first band gap near the second band.

The lower-left diagram of Fig. 7 and the top-right diagram of Fig. 8 depict modes for frequencies in the "band-tail" regions of the disordered PhC, frequencies which lie in the gap regions for the corresponding PhC without disorder. These modes are extended over the supercell but show no Bloch wave character.

A third category of states is formed by the gap states isolated in frequency within the gap regions (as opposed to the disorder-broadened bands). The modes from this category are shown in the bottom-right of Fig. 7 (positional disorder) and at the bottom of Fig. 8. These states are not extended over the whole supercell, but are occupying only part of it.

4. Conclusions

The effect of disorder acting on a PhC to the band structure of electromagnetic waves is a narrowing of the photonic band gaps and additionally the appearance of states within these gaps. The states with frequencies within the photonic bands — the band states — even in the absence of disorder are distorted but retain their Bloch wave character. This character is lost for the tail states —

states with frequencies which lie in photonic bands only due to the disorder induced gap narrowing. Nevertheless, the tail states are still extended. A third category of states — gap states — is induced within the narrowed gaps. These states are localized within limited regions of the PhC. Positional and radial disorder both show this effect. The difference is quantitative — the distance of the displacement (determined by positional disorder parameter δ_{p}) has to be relatively far larger than the change in size (radial disorder parameter δ_{r}) to have a comparable effect.

Acknowledgments

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