

The effect of disorder on the local density of states in two-dimensional quasi-periodic photonic crystals

C Rockstuhl¹ and F Lederer

Institute of Condensed Matter Theory and Solid State Optics,
Friedrich-Schiller University Jena, Max-Wien Platz 1, 07743 Jena, Germany
E-mail: carsten.rockstuhl@uni-jena.de

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Abstract. We analyse the effect of disorder in radius, dielectric constant and spatial position of high refractive index cylinders, forming several types of quasi-periodic photonic crystals, on its local density of states (LDOS). We focus on the two lowest frequency regions where the LDOS is small for TM-polarized light, where the electric field is parallel to the cylinder axis. It turned out that these spectral regions are almost independent of the strength of position disorder but vanish quickly for the two other disorder types. Hence, we conclude that in such crystals the spectral domains with small LDOS are primarily associated with Mie resonances of a single cylinder. This behaviour is compared to a photonic crystal made of air holes in a high refractive index background medium, a structure where Bragg reflection evokes band gaps.

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¹ Author to whom any correspondence should be addressed.

1. Introduction

Back in the mid-1980s x-ray diffraction patterns of metallic alloys were observed, which did not fit into those of any well-known crystallographic symmetry classes. Based on these findings Levine and Steinhardt proposed a new type of symmetry group, now frequently termed quasi-periodic structure [1]. In contrast to a Bravais lattice, the proposed structure lacks translational symmetry. Instead it exhibits a particular rotational symmetry which leads to its classification. While Bravais lattices possess only 2-, 3-, 4- and 6-fold symmetries, any other rotational symmetry larger than unity can be found in quasi-periodic structures.

Soon after this terminology was proposed for crystalline materials, the concept was extended towards artificial photonic materials. Quasi-periodic photonic structures in one [2], two [3, 4] and, more recently, three dimensions [5] have been proposed and experimentally investigated. The main emphasis was on searching for spectral domains with low values in the local density of states (LDOS), a phenomenon well-known for genuine photonic crystals (PC) exhibiting translational symmetry where gaps appear in the band structure. Band gaps are associated with a LDOS that is zero. Field propagation is prohibited for frequencies situated in these gaps of the dispersion relation [6, 7]. We note that a band structure for a QPC cannot be defined. The formation of band gaps in PCs can be explained by two physical mechanisms. For two-dimensional photonic structures made of either material cylinders in air or air holes in a dielectric host, one gap formation process is based on Mie resonances of the single cylinder [8], while another one is related to Bragg reflection at consecutive periods of the structure. In the momentum (or reciprocal) space the scattered light at these periodic structures exhibits a set of discrete peaks. As the reciprocal space of quasi-periodic photonic crystals (QPC) is likewise sparsely filled with some distinctive peaks, the formation of spectral domains with small LDOS is usually also explained with the latter mechanism. These peaks hint at a short-range order typical for QPCs [9]. This short-range order appears because the entire space filling in QPCs is obtained with a finite number of geometrical unit cells whose side lengths are equal, say a . For example, a 5-fold QPC in the 2D space can be composed of two different rhombi and a 7-fold QPC is composed of three such elements. Adopting such a scheme it may be concluded that PCs are a particular subset of QPCs, where only a single geometrical unit cell is required for obtaining complete space filling.

The role Mie resonances play in the gap formation process in PCs has been understood in analysing the effect of disorder [10, 11]. In the present paper we shall take advantage of this concept to reveal the physical origin of the spectral domains with low LDOS for QPCs. We shall concentrate on 5-fold, 6-fold, that is a classical PC with a triangular lattice, and 7-fold QPCs and focus on QPCs made of high index cylinders surrounded by air and illuminated with TM polarized light (electric field parallel to the cylinder axis). TM polarization was chosen because it provides the largest extension of the spectral domain with small LDOS for this type of photonic structures. We shall restrict ourselves to the two lowest frequency domains with small LDOS and show that they will be insensitive to position disorder but sensitive to disorder in radius and dielectric constant. For a 6-fold QPC the results will be compared to the opposite case of air holes in a high dielectric ambient medium illuminated with TE-polarized light (magnetic field parallel to the cylinder axis). In such a structure the formation process of spectral domains with small LDOS is based on Bragg reflections and correspondingly the widths of those spectral domains are equally sensitive to disorder in position and radius.

For the first time to the best of our knowledge we shall prove that for QPCs made of material cylinders in air the first two low-frequency regions with small LDOS are dominantly associated

with resonances in the single scatterer and that the actual short-range order has no significant influence. This conclusion can be drawn from the disorder analysis. We shall outline the necessary numerical details of the computational procedure in section 2, present the results in section 3 and discuss them in section 4.

2. Numerical procedure

A grid formalism was employed for the generation of the local position of the cylinders, which form the QPC in the unperturbed case [12]. We employed a self-consistent multiple scattering formalism for solving the interaction problem of the structure with the illuminating field and for calculating the LDOS [13]. In preliminary numerical experiments it was verified that for an unperturbed QPC the exact position of the line source within the QPC has no influence on the unambiguous determination of the region with small LDOS in the particular structure. Only the appearance of defect modes in the LDOS of QPCs due to local configurations with two or more closely spaced cylinders depends on the chosen position of the line source [14]. These defect modes appear as sharp spectral peaks in the LDOS. They are a generic intrinsic property of QPCs and cannot be eliminated. A detailed analysis of them will appear elsewhere. The QPCs were assumed to have a circular shape with a radius of $R = 6a$, where a is the lattice constant of the QPC. The dielectric constant of the cylinders in the configurations without disorder is assumed to be $\epsilon_0 = 13$ and the radius of the cylinders is $r_0 = 0.2a$. In all cases analysed here the line source emits TM-polarized light. Examples for the LDOS along with sketches of the geometry of the unperturbed QPCs are shown in figure 1. It can be seen that two regions with small LDOS appear for the present system nearly independent of the structural arrangement. The first large spectral region opens between $f = 0.254a\lambda^{-1}$ and $f = 0.428a\lambda^{-1}$, whereas a second smaller spectral region opens between $f = 0.534a\lambda^{-1}$ and $f = 0.575a\lambda^{-1}$. The strength of the remaining LDOS inside these spectral domains decays exponentially with the spatial extension of the QPC [9].

Disorder was introduced in the dielectric constant of each cylinder ϵ_i as uniformly distributed random fluctuations with $\epsilon_i = \epsilon_0 + \delta_\epsilon \rho_i$, where δ_ϵ is a measure for the strength of the disorder and ρ is a random variable chosen in the interval $[-0.5; 0.5]$. In neither case a dielectric constant less than unity was generated. Likewise disorder in position was generated for the x - and y -coordinate of the centre of each cylinder. We explicitly excluded a spatial overlap of the cylinders as required for the applicability of the multiple scattering formalism. Similarly, disorder in radius was introduced where again a spatial overlap among neighbouring cylinders was excluded. The procedure for generating the actual disordered distribution consisted therefore of, firstly, choosing randomly a certain QPC cylinder and, secondly, determining its variation in position, radius or dielectric constant depending on the type of disorder studied. The procedure is iteratively repeated until a configuration is found where the above restrictions are fulfilled. Likewise the parameters of all cylinders forming the QPC were determined. For each strength of disorder δ 20 different configurations were evaluated and the resulting LDOSs were averaged.

3. Results

3.1. Disorder in radius

The LDOS in the vicinity of both relevant spectral domains for which the LDOS takes low values is shown as a function of radius disorder for the 7-fold QPC in figures 2(a) and (b), for the 6-fold

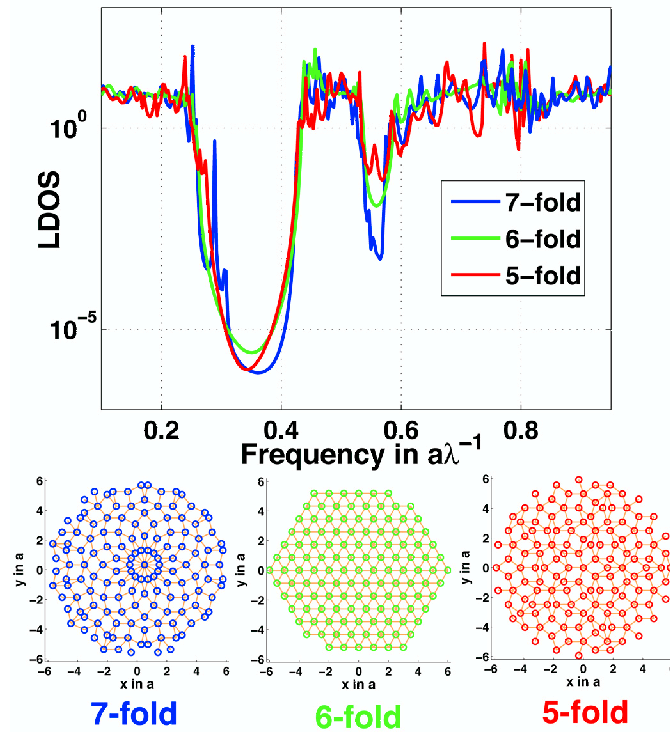


Figure 1. LDOS for 5-, 6- and 7-fold QPCs. The structures are shown in the lower part of the figure where the line source is located at the centre of the coordinate system. The QPCs are composed of cylinders with $\epsilon_0 = 13$ and a radius of $r_0 = 0.2a$. The line source is TM polarized.

QPC in figures 2(c) and (d) and for the 5-fold QPC in figures 2(e) and (f), respectively. The LDOS is plotted on a logarithmic scale with black denoting a low and white a large value. This type of presentation was chosen because the existence of defect modes in the LDOS complicates the proper identification of the exact spectral domain where the LDOS is small if disorder is involved. Again, these defect states manifest themselves as a spectrally narrow increased LDOS.

Both spectral domains with small LDOS get narrower with increasing disorder. For the first spectral domain the central frequency remains almost constant and a continuous increase (decrease) of the lower (upper) frequency of the spectral domain with small LDOS can be observed. For the second frequency domain with small LDOS the upper edge frequency remains nearly constant and the lower edge frequency increases with increasing disorder. The strength of disorder where the first frequency domain with small LDOS vanishes amounts to $\delta_{\text{Radius}} \approx 0.12a$ for all three kinds of QPCs. Likewise the strength of disorder, where the second frequency domain with small LDOS vanishes completely, is independent of the QPC type and is $\delta_{\text{Radius}} \approx 0.03a$.

3.2. Disorder in position

Next we analysed disorder in the position of the cylinder centres. The LDOS in the spectral domain around the two spectral regions with small LDOS are shown in figure 3 for the 7-fold (a and b),

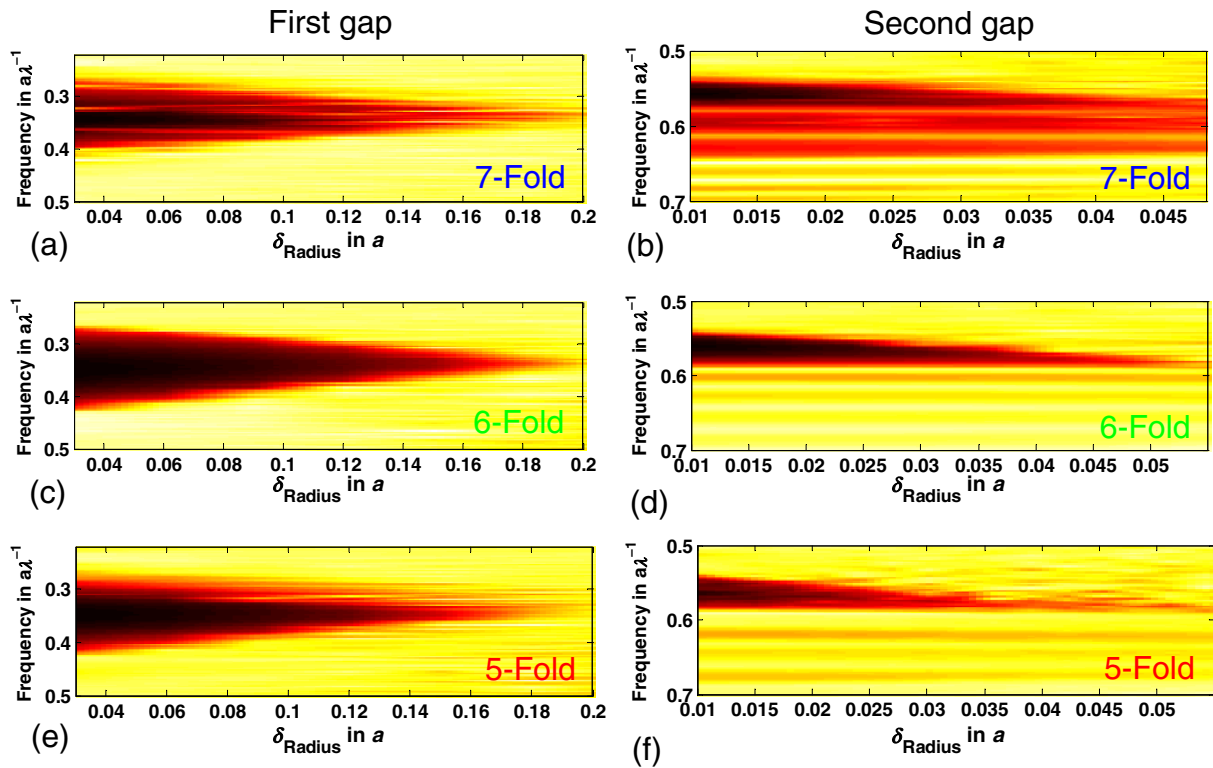


Figure 2. LDOS for a 7-fold (a and b), 6-fold (c and d) and 5-fold (e and f) QPC as a function of radius disorder in the vicinity of the two regions with small LDOS.

the 6-fold (c and d) and the 5-fold (e and f) QPC. The first spectral domain with small LDOS between $f = 0.254a\lambda^{-1}$ and $f = 0.428a\lambda^{-1}$ is highly resistant against positional disorder.

An example of a strongly perturbed 6-fold QPC is shown in figure 4(a). Actually, the degree of disorder ($\delta_{\text{Displ.}} = 1a$) is the highest achievable one. Here each cylinder is randomly displaced within a unit cell. There is almost no spatial overlap between the ideal and this strongly perturbed QPC and the structure can be regarded rather as a random photonic material. This causes a saturation of the possible disorder at the largest possible value and a further increase of the displacement of each cylinder will not cause a significant change in the LDOS.

QPCs subject to such a strong disorder do not exhibit any rotational or translational symmetry but show still spectral domains with small LDOS. At saturation of the disorder the width of the spectral domain with low values in the LDOS is largest for the 6-fold and smallest for the 7-fold QPC. This can be explained by defect states appearing in the LDOS because of almost touching or, on the other hand, missing cylinders in certain QPC domains. For sufficiently strong position disorder these defect modes appear regularly spaced and cause a shrinkage of the spectral domain with small LDOS. For nearly touching cylinders, acceptor modes in the LDOS of the QPC are created causing an increase of the lower frequency that terminates the spectral domain with small LDOS. This is comparable to the generation of acceptor modes in a PC, where those modes are lifted from the dielectric band into the gap. Missing cylinders introduce donor modes near the upper frequency of the spectral domain with small LDOS, thus decreasing effectively the upper

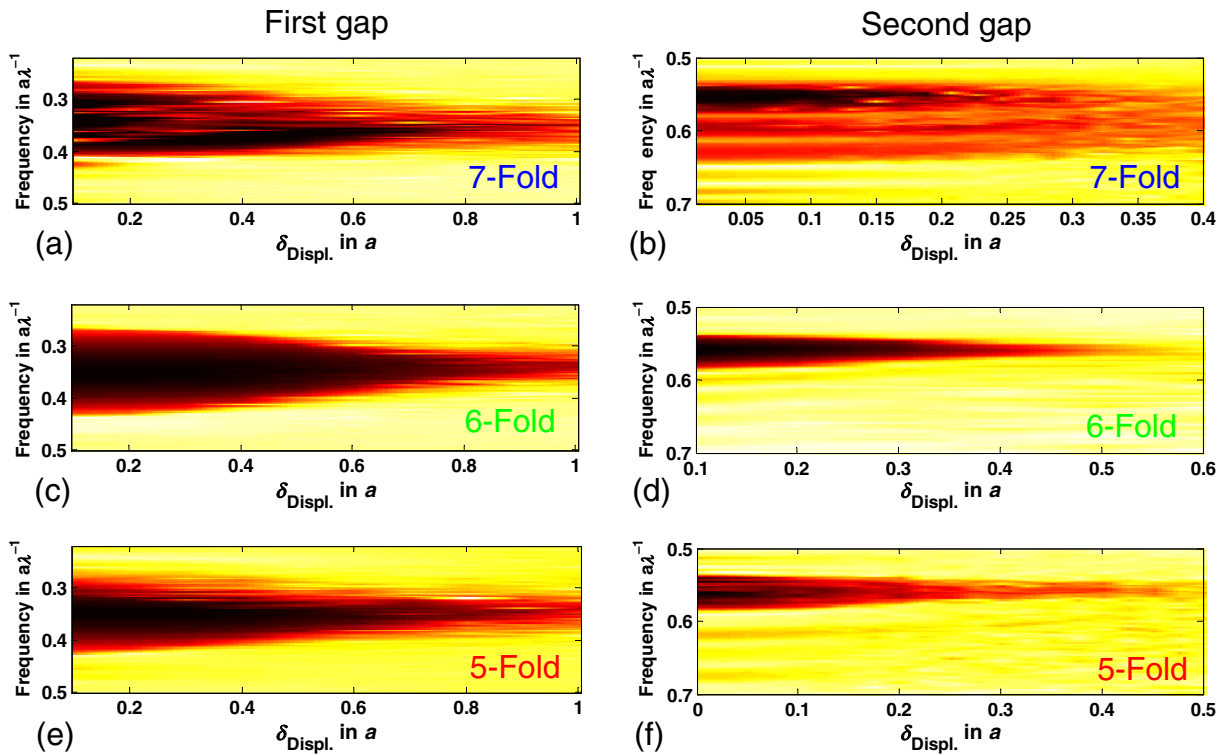


Figure 3. LDOS in the spectral vicinity of the two regions with small LDOS as a function of the position disorder of the cylinders for a 7-fold (a and b), 6-fold (c and d) and 5-fold (e and f) QPC.

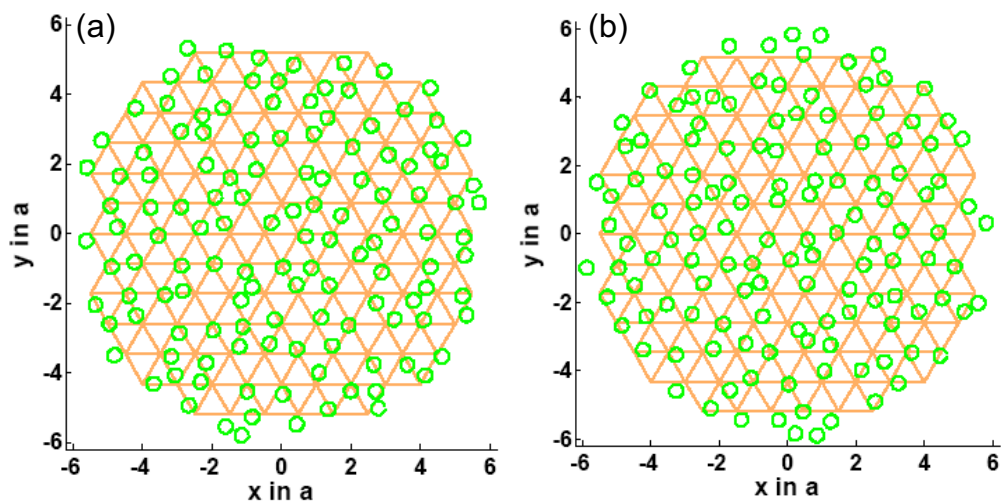


Figure 4. Examples of strongly perturbed 6-fold QPC in position where the spectral domain with small LDOS vanishes in (a) for the first spectral domain and in (b) for the second spectral domain. The underlying grid serves as a guide to the eye showing the unperturbed QPC.

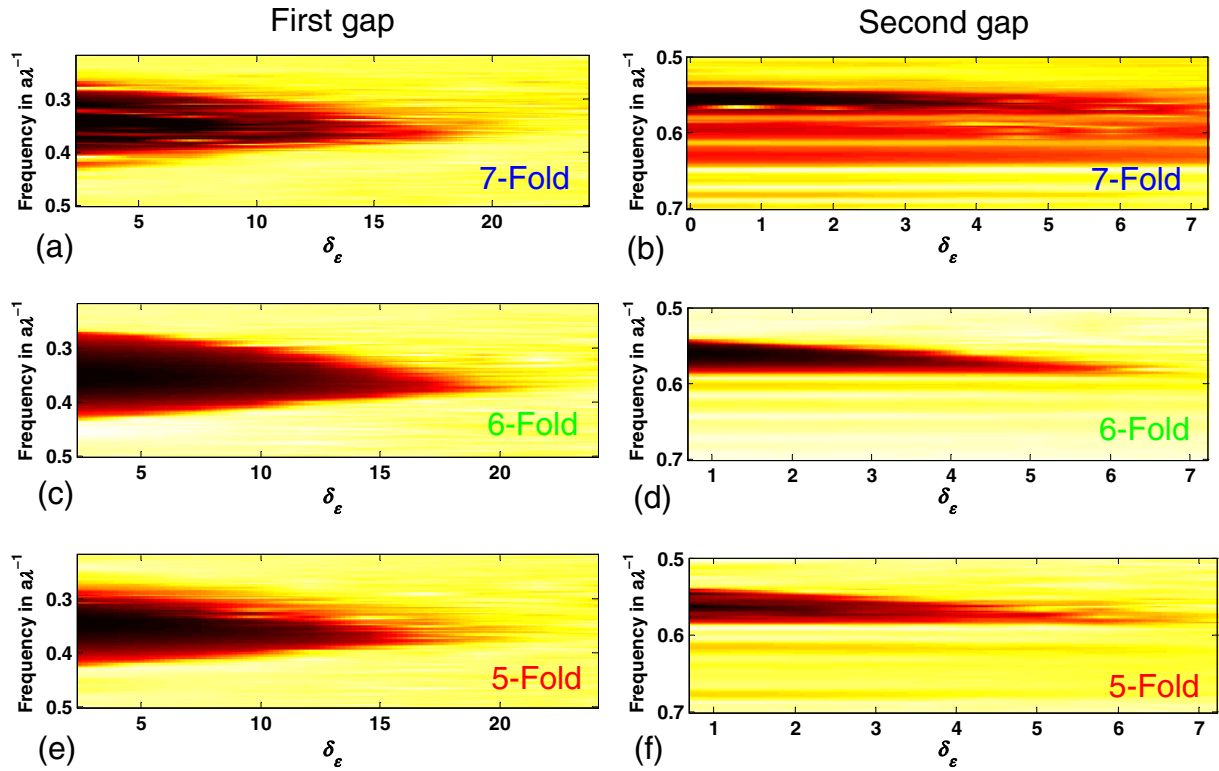


Figure 5. LDOS in the spectral vicinity of the two regions with small LDOS as a function of the disorder in the dielectric constant of the cylinders for a 7-fold (a and b), a 6-fold (c and d) and a 5-fold (e and f) QPC.

frequency of the spectral domain with small LDOS. Because the cylinder density is highest for the 7-fold QPC the probability of touching each other is also highest. Hence, more acceptor modes appear and the shrinkage of the spectral domain with small LDOS is mainly due to the increase of the lower frequency that terminates the spectral domain with small LDOS. For a 6-fold QPC donor and acceptor modes have almost the same effect and shrinkage of the spectral domain with low values in the LDOS appears symmetrically.

Generally, the same observations are made for the second spectral domain with low values in the LDOS. The 6-fold QPC shows the highest resistance against position disorder, where up to a disorder parameter $\delta_{\text{Displ.}} \approx 0.3$ the spectral domain with small LDOS survive whereas the 7-fold QPCs cease to form spectral domains with small LDOS for $\delta_{\text{Displ.}} \approx 0.15$. For all three QPCs the shrinkage of the spectral domain with low values in the LDOS manifests itself by an increase of the lower frequency and a decrease of the upper frequency that terminate the spectral domain with small LDOS. It is interesting to note that the fine structure in the LDOS of a 7-fold QPC for frequencies $f > 0.575a\lambda^{-1}$ is likewise perturbed by disorder of such a strength. This was not observed for disorder in radius and represents a precursor of weak localization in QPCs.

3.3. Disorder in dielectric constant

Finally, disorder in the dielectric constant of each single cylinder was analysed. The LDOS in the spectral vicinity of the two frequency domains with small LDOS is shown in figure 5 for the

Table 1. Evaluated disorder parameter α for each analysed QPC as a function of the disorder type for which the first and second frequency domain with small LDOS vanishes.

Type	7-fold		6-fold		5-fold		Inverse 6-fold	
	1st	2nd	1st	2nd	1st	2nd	1st	2nd
Radius	6.0	1.6	7.2	2.2	6.2	1.5	0.82	0.33
Position	16.1	7.0	22.4	15.9	18.5	7.4	0.81	0.31
ϵ	3.9	0.65	4.5	1.1	4.1	0.82	–	–

three pertinent QPC types. The increase of disorder causes a monotonous decrease of the size of the first spectral domain with low values in the LDOS, whereas the lower (upper) frequency that terminate the spectral domain with small LDOS continuously increases (decreases). The strength of disorder where the spectral domain with small LDOS tends to disappear is comparable for all three QPC types. While the first spectral domain with small LDOS is still noticeable at a disorder of $\delta_\epsilon \approx 13$, the second spectral domain with small LDOS already vanishes at $\delta_\epsilon \approx 2$ where this value is slightly larger for the 6-fold QPC.

4. Discussion

For comparing the influence of various types of disorder we introduce a generalized disorder parameter α [11]. It is a measure of the effect of disorder on the dielectric function of the photonic structure. This measure is useful because this single parameter characterizes the strength of disorder of the detailed dielectric function of which enters the computational procedure. The disorder parameter α is determined by evaluating a rms value of the disordered dielectric function $\epsilon_{\text{Dis}}(x, y)$ by any of the three types of disorder as compared to that of ideal QPC $\epsilon_0(x, y)$ using

$$\alpha = \sqrt{\frac{1}{A_{\text{QPC}}} \int_{A_{\text{QPC}}} dx dy (\epsilon_{\text{Dis}}(x, y) - \epsilon_0(x, y))^2},$$

with A_{QPC} being a square of side length $14a$ including the entire QPC. The parameter was evaluated for each simulated configuration of QPC subject to a certain disorder and subsequently the mean was taken. Table 1 shows the parameter α where the first and second spectral domains with a small LDOS vanishes for each type or disorder and for each of the three types of analysed QPCs. Note that these values are subject to a certain uncertainty, because the exact strengths of disorder for which the spectral domains with small LDOS disappear are hardly decidable. It is important to note that the strength of disorder that causes a shrinkage and ultimately a vanishing of the spectral domain with small LDOS are comparable for disorder in radius and dielectric constant. This holds for both the respective first and the second spectral domain. In contrast, these domains persist a significantly stronger disorder in position. Here, the allowed maximum strength could not be determined for the first spectral domain of the 5- and 6-fold QPCs due to the saturation of the achievable disorder. A further increase of the introduced disorder δ_{Displ} did not cause a further change in α . The respective second spectral domain withstands a factor-of-five stronger disorder than that in radius or dielectric constant. These differences can be explained

if the formation of domains with small LDOS is primarily attributed to Mie resonances of the single cylinders as the underlying physical mechanism.

In Mie theory all emerging fields, namely incident, scattered and transmitted ones, are expanded in the vicinity of the cylinder into an orthonormal set of modes in a cylindrical coordinate system using Bessel and Hankel functions. The amplitude of each mode can be analytically determined by obeying the electromagnetic boundary conditions [15]. For TM-polarized fields they require the continuity of the electric field and its normal derivative across the cylinder surface. Mie resonances for each mode appear if the associated coefficient tends to be singular. As all modes are leaky, this condition can only be fulfilled to a good approximation. Usually, for cylinders with a size comparable to the wavelength, only a few expansion coefficients are needed in order to represent all fields near the cylinders with sufficient convergence. In particular, only a single coefficient is required for small cylinders. If the denominator of this coefficient becomes close to zero, the amplitude is enhanced and the phase changes by π if the frequency passes the resonance. At frequencies slightly above resonance, the incident field is repelled by the cylinder and the light propagation through a structure composed of these cylinders is inhibited. Details of an analysis of this process is published elsewhere [16]. The Mie resonance of the first amplitude coefficient appears for the present cylinder with a radius of $R = 0.2a$ at $f = 0.21a\lambda^{-1}$ and corresponds to a good approximation to the spectral position of the first spectral domain with small LDOS. Their exact position depends on the chosen type of QPC, hence the spatial arrangement will have a minor influence too. The same process applies principally to the second spectral domain with small LDOS. The Mie resonance frequency of the second-order amplitude coefficient is $f = 0.50a\lambda^{-1}$. The actual spectral domain with small LDOS appear at frequencies slightly larger than the Mie resonances because the phase of the scattered field fits better that of the incident wave in this spectral domain for having a phase difference of π .

Any disorder in radius or dielectric constant will primarily influence the scattering properties of each single cylinder and cause a statistical distributed Mie resonance around the central resonance frequency. For larger radii and larger dielectric constant for the cylinder the resonance frequency gets lower, whereas smaller values for both parameters causing a higher resonance frequency. As the physical impact for these both types of disorder is the same (e.g. changing the spectral position of the Mie-resonance), the spectral domain with small LDOS withstands the same strength of disorder α as observed, although slightly smaller values for disorder in the dielectric constant are necessary to cease the spectral domains with low values in the LDOS. This can be seen in table 1. If the QPC is composed of cylinders that do not support sufficient field repulsion at their surfaces, a propagation channel for the light through the structure is provided and the spectral domain with low values in the LDOS gets narrower and vanishes ultimately. The second spectral domain with small LDOS shows a higher sensitivity against disorder, because the second order Mie resonance is more pronounced and sharper as compared to the resonance connected to the first spectral domain with small LDOS.

For position disorder, the scattering properties of the single cylinder are not altered and the spectral domains with small LDOS survive for rather strong disorder. The process is limited by the necessity that no additional defect modes are excited by closely spaced or missing cylinders. These defect modes cause a shrinkage of the spectral domain with small LDOS as outlined in subsection 3.2. The results are consistent with observations reported in the literature for regular PCs [11, 17].

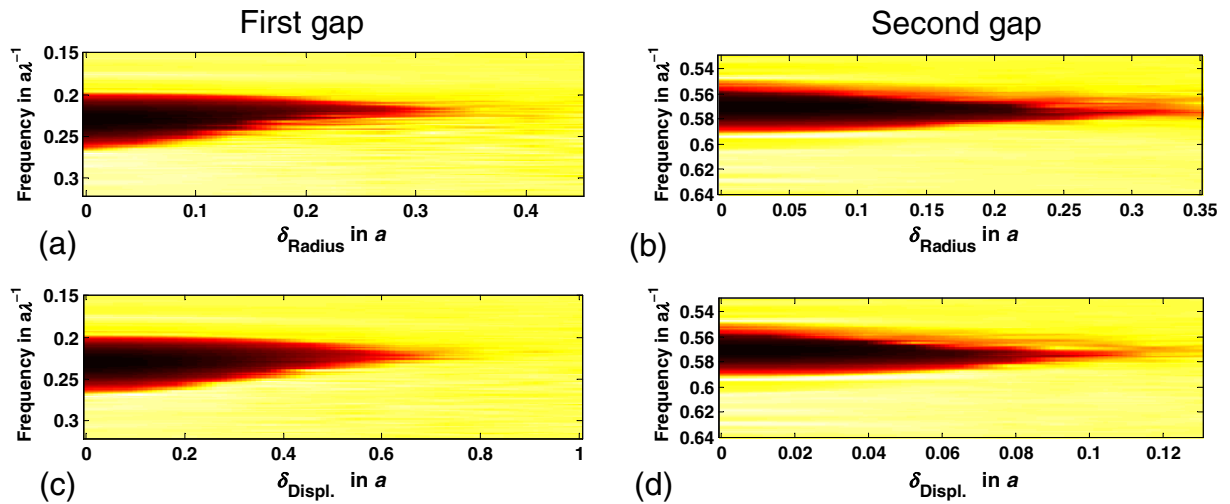


Figure 6. LDOS for a 6-fold QPC that consists of air cylinders ($R = 0.3a$) in a dielectric host medium ($\epsilon = 13$) as a function of the disorder in radius for (a) the first, (b) the second spectral domain with small LDOS and as a function of position disorder for (c) the first, (d) the second spectral domain with small LDOS.

For comparison, figure 6 shows the LDOS for an inverse 6-fold QPC where the radius of the air cylinders is $r_0 = 0.3a$. The cylinders are embedded in a background media with $\epsilon_0 = 13$ and the light emitted by the line source is TE-polarized (magnetic field parallel to the cylinder axis). The QPC has the same size as before. The particular configuration was chosen as it supports the largest spectral domain with small LDOS for an inverse structure at a given radius for the air cylinders. The figure shows the LDOS in the vicinity of the first two spectral domains with small LDOS as a function of disorder in cylinder position and radius. Results for disorder in the dielectric constant were not calculated because such a type of disorder is physically not reasonable for air cylinders in a host medium. From table 1 it can be seen that the spectral domains with small LDOS vanish independent of the type of disorder for rather low strengths at $\alpha \approx 0.8$ for the first, and at $\alpha \approx 0.3$ for the second spectral domain with low values in the LDOS, respectively. In contrast to the previous structure this QPC does not exhibit Mie resonances. The spectral domain with small LDOS are associated with Bragg reflection. By introducing disorder Bragg resonance frequencies are locally altered and this prevents the formation of a global spectral domain with small LDOS for the QPC. The process is mediated by both types of disorder, in stark contrast to the previously analysed structures, where the formation process of the spectral domains with small LDOS is primarily based on Mie resonances.

5. Conclusions

In this work we analysed the influence of disorder on the first two spectral domains with small LDOS that appear in various kinds of QPCs. It was shown that formation of those spectral domains with small LDOS is sensitive against disorder in cylinder radius and dielectric constant but insensitive against position disorder. This holds for both spectral domains. The behaviour was

explained employing Mie resonances as the dominating origin for the formation process of the spectral domain with small LDOS in a QPC that consists of high index cylinders surrounded by air for TM-polarized light. It was shown that for an inverse structure and TE-polarized light, the spectral domains with small LDOS are equally sensitive against disorder in radius and position, a typical response for spectral domains with low values in the LDOS whose origin is traceable to the Bragg effect.

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