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Disorder induced modification of reflection and transmission spectra of a two-dimensional photonic crystal with an incomplete band-gap

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Abstract
Transmission and reflection of light in disordered two-dimensional photonic crystals with an incomplete photonic band-gap have been modelled for various levels of disorder. It is found that ballistic and scattered light display different behaviours as a function of the disorder parameter. For ballistic light, the dependence of the transmission coefficient on the disorder parameter exhibits a threshold-like behaviour, whereas the transmission of scattered light increases rapidly for small disorder. Unlike for photonic crystals with a complete band-gap, the minimum of the transmission for scattered light does not coincide with the centre of the photonic band-gap, and Fabry–Perot-type oscillations can be seen within the photonic band-gap.

Photonic crystals [1, 2] have recently been the subject of much research due to the potential applications arising from their ability to confine, manipulate and guide light, and also for the potential to inhibit spontaneous emission. Most of these applications rely on the existence of a photonic band-gap (PBG), which can result from the periodic variation of the refractive index that photonic crystals possess.

However, in real photonic crystals, this perfectly periodic variation of refractive index is disturbed to some extent by the presence of disorder. The disorder can take different forms. For example, in three-dimensional photonic crystals based on self-assembled opal structures [3, 4], the radius of the spheres will show some dispersion, and there will be lattice vacancies and stacking faults [5]. In two-dimensional photonic crystals formed by the etching of air cylinders into a semiconductor substrate, the radius of the cylinders can again show dispersion, the

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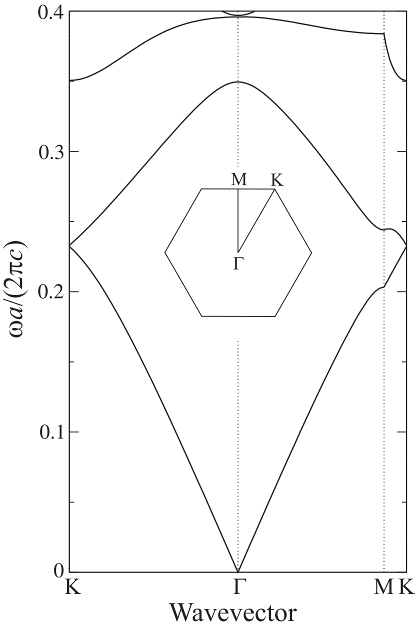

Figure 1. Band structure of the ideal photonic crystal for the TM polarization. The band structure was calculated using the plane wave method, using a basis set of 4291 plane waves. Inset—the hexagonal first Brillouin zone for the ideal photonic crystal.

cylinder centres can lie away from the ideal lattice locations of the crystal and the walls of the etched semiconductor will normally display a certain surface roughness.

Disorder in photonic crystals is of interest for a number of reasons. For example, the possibility of light localization due to disorder in photonic crystals is of fundamental interest and could find applications. Also disorder can damage the PBG by partly or completely filling it with localized states, and since most potential applications of photonic crystals rely on the PBG, this could lead to the unsuitability of the crystal for certain devices.

This paper reports a study of the effect of a certain type of disorder on a two-dimensional photonic crystal with an incomplete band-gap. The ideal photonic crystal considered consists of air cylinders of radius $0.4a$ (where a is the lattice constant, or the distance between the centres of neighbouring cylinders) etched into a GaAs substrate ($\varepsilon = 12.96$) and arranged on a hexagonal lattice of points. The crystal possesses a wide, complete PBG for the TE polarization [6]. (The TE polarization has its electric field in the plane of the variation of refractive index, whereas the TM polarization has its magnetic field in this plane.) Figure 1 shows the band structure for the TM polarization of the ideal photonic crystal, calculated using a plane wave method [6–8]. For the TM polarization, a PBG exists for the Γ–M direction of the Brillouin zone centred on $\omega a/(2\pi c) \approx 0.223$ and of width 18% relative to its centre frequency. However, this PBG narrows and eventually closes when the propagation direction is shifted toward the Γ–K direction. Hence the TM polarization in this ideal structure is suitable for studying the effects of disorder on a photonic crystal with an incomplete band-gap. The type of disorder studied here is in the form of a random shift of the centre of the air cylinders away from the ideal lattice locations and into a circle of radius δa centred on the ideal lattice location. Thus the parameter δ is a measure of the 'amount of disorder' present in the system.

This work follows previous studies of disorder in the same ideal structure [9–11]. In [9] and [10], the disorder was of the form of a random dispersion of the cylinder radii. In [11], the

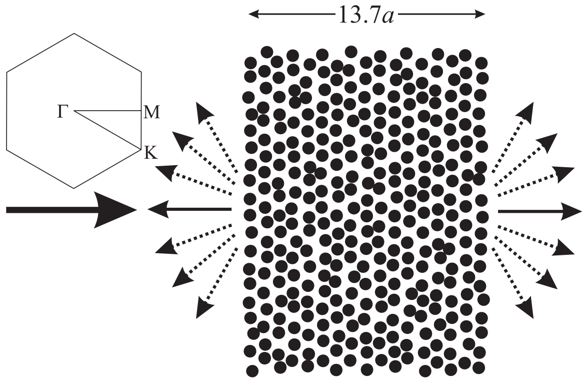

Figure 2. An illustration of the calculations undertaken. A disordered supercell is shown, and the black circles represent the air cylinders. The large arrow indicates the direction of incident light. The small solid arrows show the direction of ballistic transmission (right) and ballistic reflection (left). The dotted arrows indicate scattered transmission and reflection. Also shown is the first Brillouin zone of the ideal photonic crystal, which indicates the directions in reciprocal space.

disorder was of the same kind as considered in this paper, but in the context of transmission of light through a photonic crystal with a complete PBG (i.e. in the TE polarization). These studies all found a threshold-like behaviour with respect to the disorder parameter. For a small amount of disorder, edge states narrow the PBG but the transmission spectra do not suffer major modification. However, disorder above the threshold produces localized states throughout the PBG and the transmission of light through the photonic crystal is affected substantially. These localized states are seen to have the characteristics of 'random microcavity' modes. The threshold-like behaviour with the disorder parameter has also been found in one-dimensional photonic crystals [12].

Calculations of the transmission and reflection spectra are based on a combination of transfer matrix and multiple-scattering techniques, using a modified version of the publicly available code of Pendry *et al* [13–15]. The disordered supercell used in the calculations is shown in figure 2 and consists of 17 rows of 19 cylinders (323 cylinders in total), and each cylinder was described by a 7 by 6 mesh. Periodic boundary conditions were imposed at the top and bottom of the structure, and the sample thickness used in the modelling was $13.7a$.

In order to model the spectra of real disordered photonic crystals (which usually display smooth transmission dips in the spectral regions of PBGs), the calculations were averaged over several random configurations of disorder. The values of the disorder parameter used in the modelling were $\delta = 0.01, 0.02, 0.05, 0.1, 0.15$ and 0.2, and for each case the spectra were calculated for ten random configurations of the disordered crystal. Experimentally, the transmission spectrum of photonic crystals is usually studied in one of two ways, as illustrated in figure 2. The ballistic transmission can be measured, where the transmitted light is parallel to the incident light; or the total transmission is measured, where all the light emerging from the rear of the sample is collected, and comprises the ballistic and scattered contributions. Hence, in the modelling undertaken, the ballistic and scattered contributions to the transmitted light are considered separately. Likewise for the reflection spectra, the total reflection is separated into contributions from the specular reflection (anti-parallel to the incident light) and scattered reflection. In the modelling, light is taken as incident along the Γ–M direction of the ideal crystal's Brillouin zone in reciprocal space, as indicated in figure 2.

Figure 3 shows the calculated transmission and reflection spectra for the disorder parameters $\delta = 0.01, 0.02, 0.05, 0.1, 0.15$ and 0.2. The thin lines are for the spectra of one

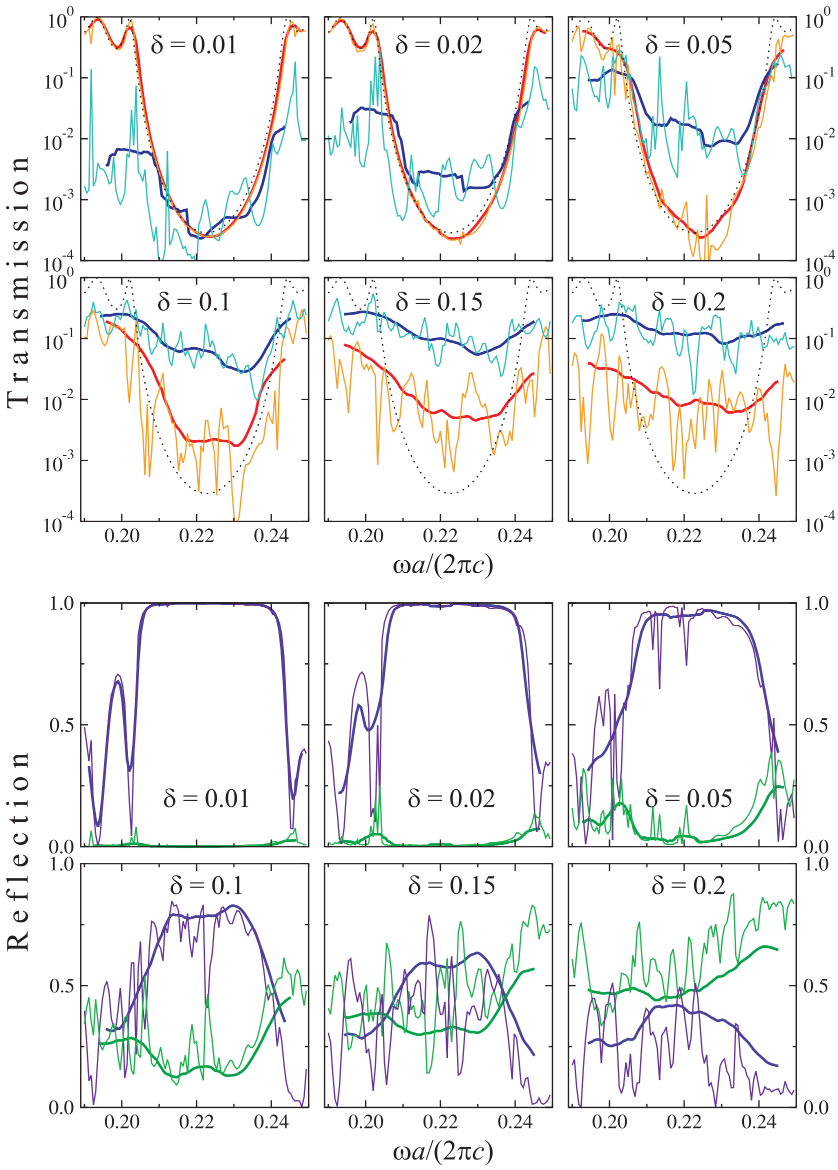

Figure 3. Top—calculated transmission spectra for disordered photonic crystals with δ = 0.01, 0.02, 0.05, 0.1, 0.15 and 0.2. Red lines are the ballistic transmission, blue lines are the scattered transmission—the thin lines for an individual configuration of disorder, and the heavy lines for the mean averaged over 10 random configurations of disorder. The ballistic transmission spectrum of the ideal photonic crystal is also shown (black dotted line) for comparison. Bottom—calculated reflection spectra for the same structures. Indigo lines are the ballistic reflection, and green lines are the scattered reflection.

individual configuration of the disorder, and the heavy lines are the mean spectra, averaged over ten random configurations of disorder and additionally smoothed to remove remaining traces of the spikes. The ballistic transmission of the ideal crystal is also shown (as a dotted black line) for comparison. The ideal crystal does not display any scattering of light, as the band-gap under study is below the diffraction cut-off of the photonic crystal.

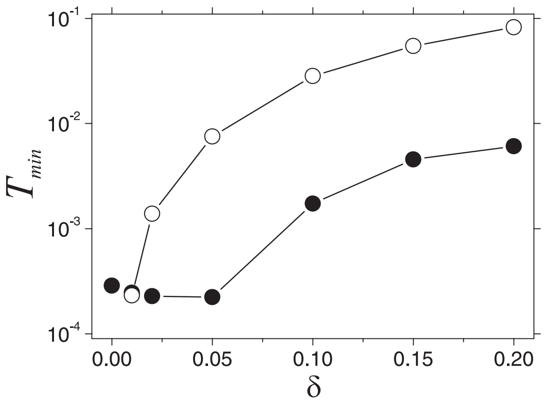

Figure 4. The transmission coefficient at the minimum (T_{min}) for ballistic light (closed circles) and scattered light (open circles) as a function of the disorder parameter δ.

As can be seen from the transmission spectra of figure 3, light incident on the ideal photonic crystal in the Γ–M direction in the spectral region of the incomplete PBG undergoes attenuation, and a symmetrical transmission dip is observed in the ballistic transmission. In contrast to the ideal case, when disorder is introduced into the photonic crystal, scattered light appears in the transmission spectrum, and the ballistic transmission becomes asymmetric. For the smallest amount of disorder considered ($\delta = 0.01$), the scattered transmission is comparable to the ballistic transmission, but for larger disorder parameters the scattered light dominates the transmission spectra. Also, for small disorder ($\delta \leqslant 0.05$), the ensemble-averaged ballistic transmission shows little deviation from that of the ideal crystal. Even so, for $\delta = 0.05$, individual configurations of disorder can show spikes in the transmission dip. It can be seen that ballistic and scattered transmission display different behaviours as a function of the disorder parameter δ. The transmission coefficient at the minimum (T_{min}) of the spectral dip in the region of the incomplete PBG is shown in figure 4. Interestingly, it is seen that for small values of the disorder parameter δ, the transmission coefficient at the minimum of the transmission dip for ballistic light can be smaller than for its ideal crystal counterpart. This is despite the fact that one might expect disorder to decrease the attenuation within the crystal, and therefore lead to more transmission. However, for this narrow, partial PBG under study, where the total attenuation of light through the crystal is small, the effect of Rayleigh scattering in the disordered crystal (which serves to remove light from the ballistic transmission) can be large enough to cause the minimum transmission to be reduced when disorder is introduced.

Figure 4 also displays the threshold behaviour found in previous studies [9–11], where the ballistic transmission changes little up to a threshold level of disorder, and then increases rapidly above that threshold.

The averaged scattered transmission spectra in figure 3 also display an asymmetric, triangular shape. The reasons for this asymmetry can be understood in terms of the following simple physical arguments based on the band structure in figure 1. Suppose light is incident on the disordered crystal in the Γ–M direction at a frequency corresponding to the incomplete PBG. In this case, an evanescent wave will be excited in the crystal, characterized by some attenuation length. Due to the disorder, the wave can be scattered into a propagating state in a direction closer to Γ–K. The wave can then proceed to the rear of the sample without further attenuation, and be transmitted. Also possible is the scattering of the incident wave into another evanescent state (as opposed to propagating state) that is closer to the Γ–K direction, and thus characterized by a smaller attenuation length (since the PBG is smaller for directions away from Γ–M; see figure 1). The direction of the shape modification depends on the details of the curvature of the band structure between the Γ–M and Γ–K directions for the photonic crystal. For the present case, the change in wavevector needed to scatter to a propagating state is smaller for higher frequencies (in the second photonic band) than for the lower frequencies (in the first photonic band), and so the shift of the minimum transmission is to higher frequencies.

The smaller shape asymmetry in the ballistic transmission can be explained by a similar reasoning. Once the incident wave has been scattered by the disorder, it can then be scattered a second time, occasionally back into the Γ–M direction where it will contribute to the ballistic transmission. This second-order effect then leads to the shift of the minimum in the transmission away from the centre of the PBG.

Usually, experimental studies assign the centre of the PBG of real photonic crystals to the minimum of the transmission spectrum. However, when scattered light is dominant in the total transmission, the shape asymmetry discussed above means that the minimum of the total transmission will depend on the details of the band structure of the photonic crystal, and does not correspond to the centre of the PBG. Simply assigning the centre of the PBG to the minimum of the transmission through the crystal can thus lead to significant error in (disordered) photonic crystals with an incomplete PBG.

When light is scattered into propagating modes away from the incident Γ–M direction, it is free to propagate through the photonic crystal without attenuation. Thus the light will experience multiple reflections in the crystal, and this leads to Fabry–Perot oscillations in the transmission spectra for scattered light in the spectral region of the incomplete PBG, which can be seen in figure 3. From the scattered transmission spectra for individual configurations of disorder, it can be seen that these Fabry–Perot oscillations have a similar period to the Fabry–Perot oscillations outside the PBG for the ballistic transmission. In fact, the spectral period of the Fabry–Perot oscillations is inversely proportional to the path length of the light through the structure, and thus is proportional to a factor of $\cos\alpha$, where α is the angle of propagation relative to the surface normal. The Fabry–Perot oscillations in the scattered transmission within the PBG are due to light scattering from evanescent waves in the incident Γ–M direction into propagating waves closer to the Γ–K direction. Thus $\alpha \leqslant 30^\circ$, and the difference between the period of the Fabry–Perot oscillations in the ballistic transmission outside the PBG and the width of the Fabry–Perot oscillations in the scattered transmission within the PBG is only around 10%.

These Fabry–Perot oscillations can be differentiated from the spikes caused by the localized modes. The spikes in the transmission dip are due to states being introduced into the former PBG by the disorder, and as such their spectral position and width are random in nature. This is what leads to the overall raising of the ensemble-averaged transmission. However, the oscillations observed in the scattered transmission have a more systematic nature—they are seen throughout the former PBG and differing configurations of disorder give rise to similar oscillations. Hence they are also seen in the ensemble-averaged scattered transmission, although when the scattered transmission is averaged over many different configurations, the random nature leads to a slight broadening of the oscillations, and also a decrease of their amplitude.

The observation of Fabry–Perot modes in the scattered transmission within the former PBG is a band structure related effect. It relies on the PBG closing for some direction of propagation, such that evanescent modes excited in the crystal by the incident wave can be scattered into propagating modes in directions where the modes lie outside the PBG. Thus the observation is unique to cases where the PBG is incomplete.

Figure 3 also shows the calculated reflection spectra for $\delta = 0.01, 0.02, 0.05, 0.1, 0.15$ and 0.2. For small disorder parameters ($\delta \leqslant 0.02$) the reflection spectra are very similar to that of the ideal crystal, i.e. very little scattering appears and there is a distinct stop-band in the spectral region of the incomplete PBG. For $\delta = 0.05$, the scattered reflection has begun to grow, and for individual configurations of the disorder, spikes interrupt the stop-band in the ballistic reflection spectra. These spikes lead to an overall lowering of the averaged reflection spectrum. For larger disorder parameters ($\delta \geqslant 0.1$), the stop-band of the averaged ballistic transmission begins to flatten out, and by $\delta = 0.2$, scattered light dominates the reflection, as well as the transmission, spectrum.

In conclusion, the effect of disorder on the spectra of two-dimensional photonic crystals with an incomplete PBG has been investigated. The photonic crystal consists of air cylinders etched into a GaAs substrate, arranged on a hexagonal lattice, and the disorder is of the form of a random shift of the cylinder centres away from their ideal lattice locations. In transmission it is found that the ballistic and scattered light have different behaviour as a function of the disorder parameter. The ballistic transmission is not significantly modified for small disorder, but the scattered transmission grows quickly even for small disorder. Scattered light dominates the transmission spectra within the former incomplete photonic band-gap, even for small amounts of disorder. The transmission spectrum has dips in the PBG, which becomes asymmetric for disordered photonic crystals, such that the minimum transmission does not coincide with the centre of the PBG in disordered photonic crystals with incomplete band-gaps. Fabry–Perot-type oscillations appear within the PBG dip for scattered transmitted light.

Acknowledgment

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References

[1] Joannopoulos J D, Meade R D and Winn J N 1995 *Photonic Crystals: Molding the Flow of Light* (Princeton, NJ: Princeton University Press)
[2] Sakoda K 2001 *Optical Properties of Photonic Crystals* (Berlin: Springer) ISBN: 3-540-41199-2
[3] Blanco A, Chomski E, Grabtchak S, Ibisate M, John S, Leonard S W, Lopez C, Meseguer F, Miguez H, Mondia J P, Ozin G A, Toader O and van Driel H M 2000 *Nature* **405** 437
[4] Butsch K and John S 1998 *Phys. Rev.* E **58** 3896
[5] Yannopapas V, Stefanou N and Modinos A 2000 *Phys. Rev. Lett.* **86** 4811
[6] Plihal M and Maradudin A A 1991 *Phys. Rev.* B **44** 8565
[7] Ho K M, Chan C T and Soukoulis C M 1990 *Phys. Rev. Lett.* **65** 3152
[8] Meade R D, Brommer K D, Rappe A M and Joannopoulus J D 1992 *Appl. Phys. Lett.* **61** 495
[9] Kaliteevski M A, Manzanares Martinez J, Cassagne D and Albert J P 2002 *Phys. Rev.* B **66** 113101
[10] Kaliteevski M A, Manzanares Martinez J, Cassagne D and Albert J P 2003 *Phys. Status Solidi* a **195** 612
[11] Beggs D M, Kaliteevski M A, Abram R A, Cassagne D and Albert J P 2004 *J. Phys.: Condens. Matter* **17** 1781
[12] Vlasov Y A, Kaliteevski M A and Nikolaev V V 1999 *Phys. Rev.* B **60** 1555
[13] Pendry J B and MacKinnon A 1992 *Phys. Rev. Lett.* **69** 2772
[14] Pendry J B 1994 *J. Mod. Opt.* **41** 209
[15] Bell P M, Pendry J B, Martin Moreno L and Ward A J 1995 *Comput. Phys. Commun.* **85** 306