Large scale calculations of the propagation of light in 3D photonic crystals with disorder

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Abstract

We have researched the effects of disorder on the size of the band gap of an inverse woodpile photonic crystal. The disorder is an uniform deviation on all of the pores. This deviation will vary from 0% to a maximum of 25%. For every level of disorder, we calculate ten different disorder realization from which we will derive mean band gap size and error margins. We observed that the band gap becomes smaller as the level of disorder increases until the band gap disappears. The frequency of the upper band edge remains almost stationary while the frequency of the lower band edge shifts upwards with increasing disorder. These calculations and predictions can be compared with experiments in the future.

Introduction

Nowadays a lot of research is done into photonic crystal and their properties. There is a wide variety of crystals all with there own properties and behavior. Some of these properties are common under all photonic crystals and some are specific to the type of photonic crystal. A photonic crystal is usually composed out of two materials for example air and silicon. Photonic crystals are made out of micro structures that are on the same scale as the wavelength of light. This is usually somewhere in the hundreds of nanometers. These photonic crystals are interesting because they allow us to manipulate the light[1]. Light can move through materials and this is something we can describe by using the refractive index. Usually photonic crystals are made of two materials one with a low refractive index and one with a high refractive index. In the example earlier air has a low refractive index while silicon has a high refractive index. This is special because the arrangement of the materials is periodically repeated in space on the same scale as the wavelength of light. This is why the refractive index is also a periodically repeating pattern in space.

In this paper we are concerned with the band gap of photonic crystals and how they behave under disorder. To understand this we first take the band structure. The band strucuture of a photonic crystals describes the range of wavelenghts which may or may not propagate through the crystal. The band gap is the range of wavelengths in which the light cannot exist inside the photonic crystal[1]. The band gap is a property that every photonic crystal has, although not always in the same range. This is what makes a photonic crystal special, because it allows us to manipulate light. We can for example change the speed of light with this. In this band gap the density of optical states is equal to zero, which we are going to use to investigate their behavior under disorder. The density of states describes the amount of states per frequency interval. This is mathematically represented as a density distribution.

The density of states is continuous while the density distribution is discrete.

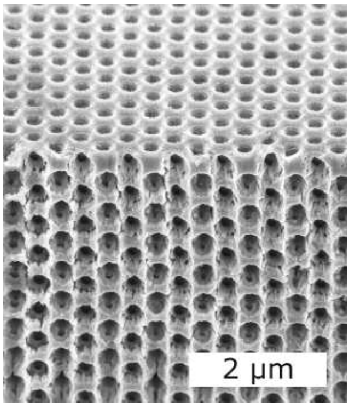

Figure 1: 3D inverse woodpile photonic crystal[7]

As mentioned before we are going to investigate what the effects of disorder are on the band gap of a photonic crystal. When creating a photonic crystal we can never create a perfect crystal. Therefore the radii of the pores will never be perfect and this is the disorder we are going to look into. We are going to investigate what happens to the band gap of a photonic crystal when all pores in the crystal have a small deviate from the optimal value. The exact model here fore will be explained later.

To do this research we are going to look into a specific photonic crystal, the inverse woodpile photonic crystal. We are going to use this photonic crystal because it has a very wide band gap[2]. This is very convenient for our research since we want to look into how the band gap behaves under disorder. To investigate this we are going to do a density of states calculation which we will revere to as DOS. The density of states shows us the frequency ranges in which light can and cannot propagate through the crystal. Under disorder we already know that the band gap will close or in other words the range of frequencies in which light cannot propagate will decrease when we increase the disorder. The main questions we want answered are how fast does it close and how does it close?

Model

To investigate these question we are going to make a model. This research will not include any experiments and is completely theoretical and computational. We used a software program named MIT photonic bandstructures or in short MPB. This program is used to compute band structures, dispersion relations and electromagnetic modes of periodic dielectric structures. This runs on both serial and parallel computers. We used this on a cluster which consists of sixteen nodes with each node having 40 processors.

Parameters

We are looking into an inverse woodpile photonic crystal. Our crystal has a length of $L = 1,5\mu m$. Furthermore these photonic crystals have a tetragonal unit cell with lattice constants (c, a, c) in the X,Y and Z directions. An inverse woodpile crystal has a lattice constant of $a \approx 500nm$ and the relations between the lattice constants is as follows $a = c\sqrt{2}$. The values that we have for L and a allow us to calculate the amount of unit cells. The amount of unit cells follow from the fraction $\frac{L}{a} = 3$. We consider a 3D photonic crystal with $3 \times 3 \times 3$ unit cells. We are looking into disorder and how the band gap reacts when we increase this disorder. The model for the disorder is based on work by Conti[3]. We use for the disorder the following equation $r = r_0(1+\gamma\xi)$. In this equation γ is the strength of the disorder. We have looked at the the following strengths of disorder thoroughly $\gamma = 0$, 0.01, 0.02, 0.05 and 0.08. This means that we have done every calculations with this disorder ten times. We have expanded these strengths of disorder with the values of $\gamma = 0.15$, 0.20, 0.22, 0.24 and 0.25. This is done because the band gap was not closed

yet. These disorders realizations have also been calculated ten times. The ξ is a uniform deviate in the interval $[-1.1]$ and $r_0 = 0.24$ is based on work done by Conti[3]. Because of the model we use for the disorder we have that the volume fraction is different in each calculation. The volume fraction is the fraction between the materials of which the crystal exist. Next to this we use $5\times5\times5$ k-points, which are vectors used to calculate the eigenfrequencies. The width of the band gap is known to be 0.136, therefore we would like a frequency resolution of $\Delta\omega = 0.15$. From Nikolaev [4] we use the following equations $\Delta\omega = \Delta k$. This would result in a k-space grid in every dimension of $\frac{1}{0.15} \approx 6\frac{2}{3}$. We round this up to 7 which results in a k-space grid of $7^3 = 343$, which covers the wanted $\Delta\omega = 0.15$. Further we know that the Brillouin zone is between the fourth and fifth band[6]. This means we need to calculate five band, because of band folding we need to calculate $5 \cdot 3^3 = 135$ bands. The last parameter is the grid resolution, we will use the resolution of $12 \times 17 \times 12$.

Results

From these calculations we have gotten the following results. In the first graph (Figure 2) we have plotted the width of the band gap against the disorder.

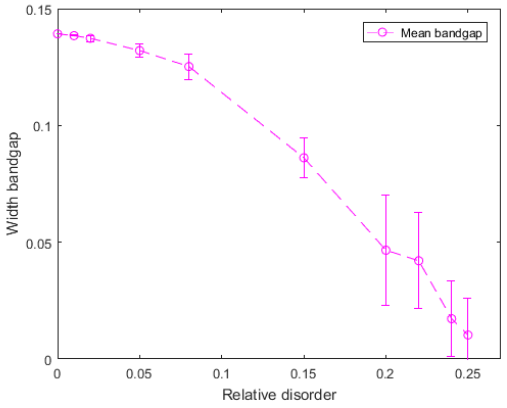

Figure 2: On the x-axis we see the disorder of the crystal. The disorder is a uniform deviate named within the bound [-1,1]. The disorder is given in terms of the maximum deviation as a fraction of the pore radius of the backbone crystal. On the y-axis we have the width of the band gap defined as the absolute band gap.

The width of the band gap is defined as the difference between the upper band edge and the lower band edge. The line that is plotted represents the mean of the band gap. We calculated every disorder realization ten times because of the uniform deviate. The circles are the average value of the band gap at a certain disorder that was calculated. The dashed lines in between the circles are interpolations of the calculated means. Furthermore we have graphed error bars on each of the calculated means. These error bars have a a length of two times the standard deviation. This means that one arm has the length of one standard deviation of the band gap. At zero disorder we have no deviation, which is visible since there are no error bars. We can also see when the disorder increases, the standard deviation increases to. This occurs as soon as we go past a certain disorder value of $\gamma = 0.20$. Then the standard deviation seems to decrease. When we look at $\gamma = 0.25$ we notice that the lower arm goes below zero. Physically it is impossible, but it

means that the band gap has been closed.

The following figure shows the mean upper and mean lower band edge.

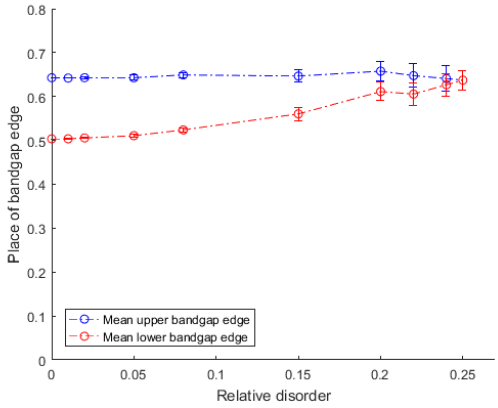

Figure 3: The lower and the upper edge of the band gap plotted as a function of the disorder. The error bars are defined as one time the standard deviation.

Again the circles are the calculated disorder values and the length of the error bars is two times the standard deviation. The lines in between the circles are interpolated. We can see that the mean value of the upper band edge stays approximately the same, while the lower band edge increases when the disorder increases. We can also see that the deviation increases when the disorder increases. At a disorder value of $\gamma = 0.25$, the mean of the lower and upper band gap are in the same place. The mean of the lower and upper band edge being in the same place does not imply that there is not a band gap. In 50% of the calculated cases there wasn't a band gap and in the other 50% there was a small band gap. That is why the mean of the lower and upper band edge seem to be they are in the same place and have an error bar.

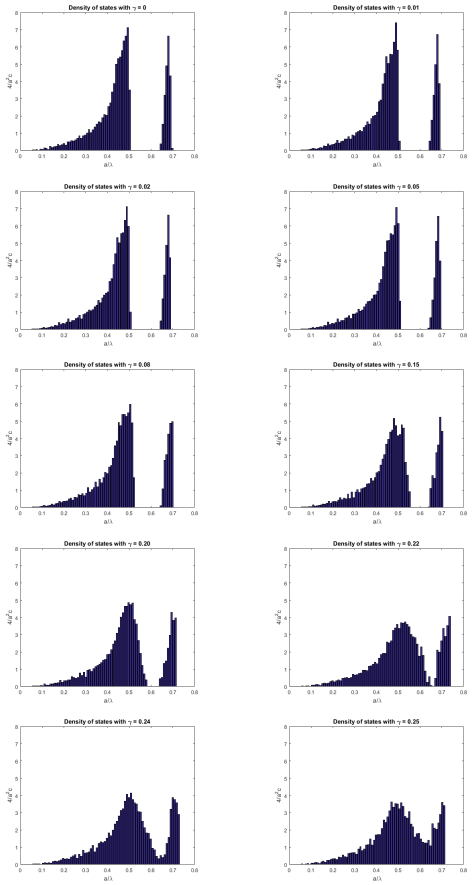

Figure 4: The first is image is with zero disorder and this is increased until the last image to $\gamma = 0.25$. On the x-axis are the reduced frequencies ranging from 0 to 0.8. On the y-axis, the density of states is scaled with the scalar $\frac{4}{a^2 c}$. The increasing of the disorder is with the same values as mentioned before.

To show the closing of the band gap further we made the density of states of one calculation at each level of disorder that we used. These are visible in figure 4. When we look at these density of states we see that the disorder increases and the band gap gets filled. The states that are on the left and right of the gap seem to go into the band gap when we increase the disorder. When we take a closer look at a single density of state we can also see something that looks like noise. To make this more clear we look at the density of states at $\gamma = 0$ in figure 5.

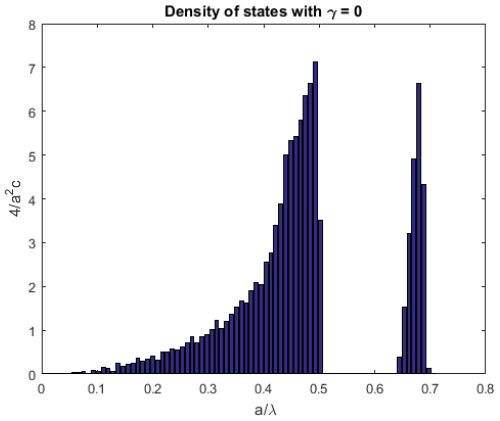

Figure 5: Density of states with $\gamma = 0$

We see that it is not a smooth curve before the band gap. This is most likely caused by the parameters we chose. We took $\Delta\omega = 0.15$ which would suggest that for our density of states we should have made bins with sizes of 0.15. We have made bins of 0.01 because the c is in practice very low and therefore we can afford to make the bins smaller. Because of the lower bin size, the density of states is not a perfectly smooth curve before the band gap.

Disorder (γ)	Standard deviation lower band edge	Standard deviation upper band edge	Standard deviation band gap
0	0	0	0
0.01	0.0005	0.0006	0.0002
0.02	0.0016	0.0028	0.0013
0.05	0.0044	0.0059	0.0027
0.08	0.0050	0.0058	0.0055
0.15	0.0150	0.0143	0.0086
0.20	0.0210	0.0211	0.0235
0.22	0.0260	0.0268	0.0206
0.24	0.0260	0.0286	0.0162
0.25	0.0218	0.0218	0.0155

Figure 6: Standard deviation of the band gap and the edges of the band gap.

To make the deviation more clear we implement the following table. In this table (figure 6) we can see all the values of the standard deviation. When we take a look at this table we can see a couple of things. The first thing to notice is that the deviation of the band gap is most of the times smaller than the deviations in the upper and lower band edge. The odd one out is at a disorder of 0.08, but there is more to that value. We saw earlier already that the deviation increases when we increase the disorder until a certain value. At an disorder of $\gamma = 0.08$ the deviation of the upper band edge is lower than the the deviation of the upper band edge at $\gamma = 0.05$. We would have expected it to be larger at 0.08 than 0.05. Furthermore when we look at the next disorder of $\gamma = 0.15$, we see that the deviation is still increasing. To explain this we look at the method we used to model the disorder. This is a uniform deviate, which means it is likely that the deviation at 0.05 is an extreme value or at 0.08 the deviation is somewhat low in comparison to what it actually should be. In other words we might have sampled smaller pore deviations by chance. Another value where the

deviation in the band gap is larger than the deviations in the lower and upper band edge is at a disorder of $\gamma = 0.20$.

The deviation of the band gap keeps increasing until we go past the $\gamma = 0.20$. This is logical because after $\gamma = 0.20$ we are encountering calculations in which the band gap has been closed. The deviation of the band edges keep increasing until $\gamma = 0.24$.

Another observation we can make is that the value of the standard deviation of the upper band edge is most of the time slightly bigger than the one of the lower band edge. If we combine this with figure 3, we can see that the upper band edge stays in approximately the same place, while the lower band edge is increasing. So the upper band edges that stays in the same place has a slightly bigger deviation than the lower band edge who increases.

A possible explanation for this is as follows. The size of the band gap can be graphed versus the size of pore radii. In this graph we get a "banana" like shaped area consisting of two curves[5,6]. At the top of this area is the curve for the upper band edge and at the bottom is the lower band edge. At the end of the banana the curve for the upper band edge does not increase much at all in comparison to the lower band edge. This explains why the lower band edge is increasing and why the upper band edge is stationary. The odd thing is that we would expect the upper band edge to have a lower deviation comparison to the lower band edge. From figure 6 we already saw the deviation of the upper band edge was slightly bigger than the lower band edge. A possible explanation for this phenomenon is possibly that there are states above the band gap, who can enter the band gap. These states always enter from the upper edge and therefore it is possible that they cause the increase in deviation in the upper band edge, especially because we have a uniform deviation in the pore radii.

Discussion

In this research there are a couple of doubts that we should address. The first thing we are going to address is the possibility to have a crystal with pore radii that have a possible deviation of 25%. We start with figure 7, which is an inverse woodpile crystal with no disorder.

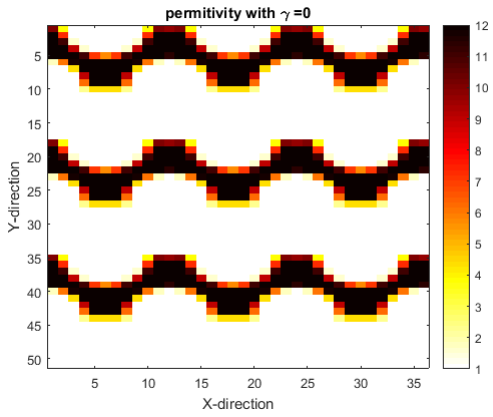

Figure 7: Inverse woodpile photonic crystal with no disorder.

This figure is a color map of the permittivity function with a perspective from one side. The white areas are the pores that are filled with air. The colored areas are the dielectric material that makes up the crystal. All the pores in this crystal are of the same radius. In figure 8 we have the same crystal only then with $\gamma = 0.25$. If we compare it with figure 7 we can see the difference in the structure, some pores are bigger while others are smaller than the pores from figure 7.

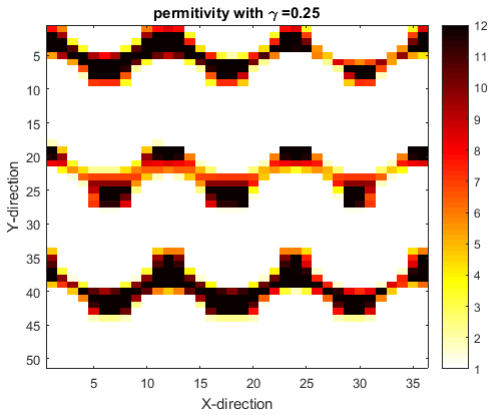

Figure 8: Inverse woodpile photonic crystal with $\gamma = 0.25$

As we can see in figure 8 the structure has changed but the crystal is possible with an $\gamma = 0.25$.

Another point of discussion is the model that we use for the disorder. It seems more logical to use a normal distribution instead of a uniform distribution for the deviation in the pore radii. The reason for not using a normal distribution is the small possibility that we get a number so big that a single pore destroys the entire crystal. A similar argument can be made for a very small number which would make the pore radius negative which is not possible. When creating a crystal in practice you never get these extreme values.. We thus want a distribution that has a bounded interval to not get these problems. Another reason for choosing a uniform distribution is that we are directly taking into account extreme cases, because they happen with equal likely hood within a uniform distribution. Therefore we can see the uniform distribution as an worse case scenario and it will only get better.

the last point is that the data we have gotten is based on a distribution. We have calculated every disorder ten times in order to reduce the effects of possible outliers. Nonetheless it is still possible that they are in the results we acquired and there is not much we can do about that except for calculating more disorder realizations. This implies that the means that we have calculated are close to the actual mean, but they can be off by a small margin.

Conclusion

In this paper we researched what happens to the band gap of an inverse woodpile photonic crystal when increasing the disorder. For this we found a couple of interesting results. We discovered how fast the band gap closes as shown in figure 1. We also discovered how the band gap closes. We saw that the lower band edge increases while the upper band edge remains in the same place. We calculated these for every level of disorder ten times with different disorder realizations and put them in graphs. We discovered that the deviation of the band gap and its edges increase with increasing disorder until we go past a certain point at which it gets smaller again. This study is completely computational and theoretical no experiments are done. The results can be used to quantitatively compare them with future experiments. Furthermore the acquired results of this research are very useful in for example creating photonic crystals. It is impossible to create a perfect crystal, but now you can make a prediction based on the precision of the creating process what the possible influences are on the crystal.

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