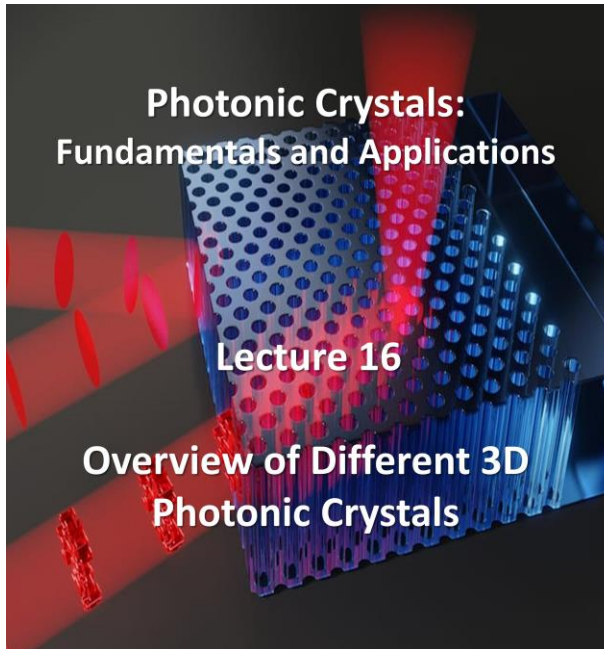


Lec 16: Overview of different 3D Photonic Crystals



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Hello students, welcome to lecture 16 of the online course on Photonic Crystals Fundamentals and Applications.



- Introduction
- 3D Photonic Crystals: Examples
- Three-Dimensional Lattices
- Dielectric Contrast of 3D Photonic Crystals
- Band Gaps of 3D Photonic Crystals
- Different types of 3D Photonic Crystals
- Spheres in a diamond lattice
- Yablonovite



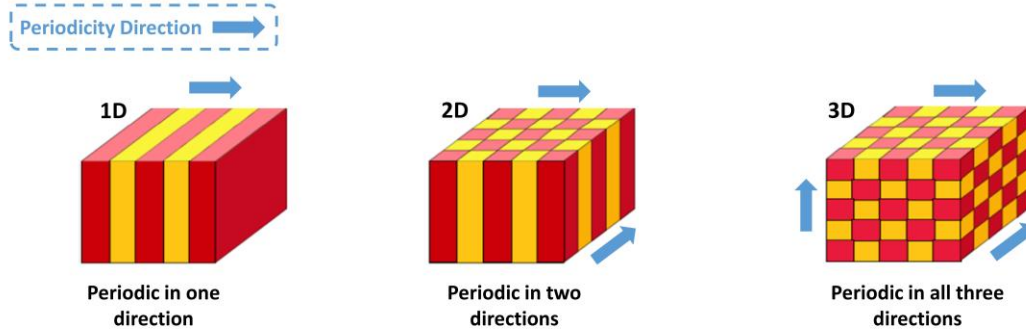
Source: J. D. Joannopoulos et al., "Photonic Crystals: Molding the Flow of Light", Princeton Univ. Press, 2008.

Today's lecture will be on the overview of different 3D photonic crystals. So, here is the lecture outline. We will have a brief introduction to the topic. We will take some examples of 3D photonic crystals, discuss about three-dimensional lattices, and we will see about the impact of dielectric contrast for the case of 3D photonic crystals and how we generate bandgaps and complete bandgaps of 3D photonic crystals. And then we will start discussing about you know different types of photonic crystals, spheres in a diamond lattice,

Yablonovite.



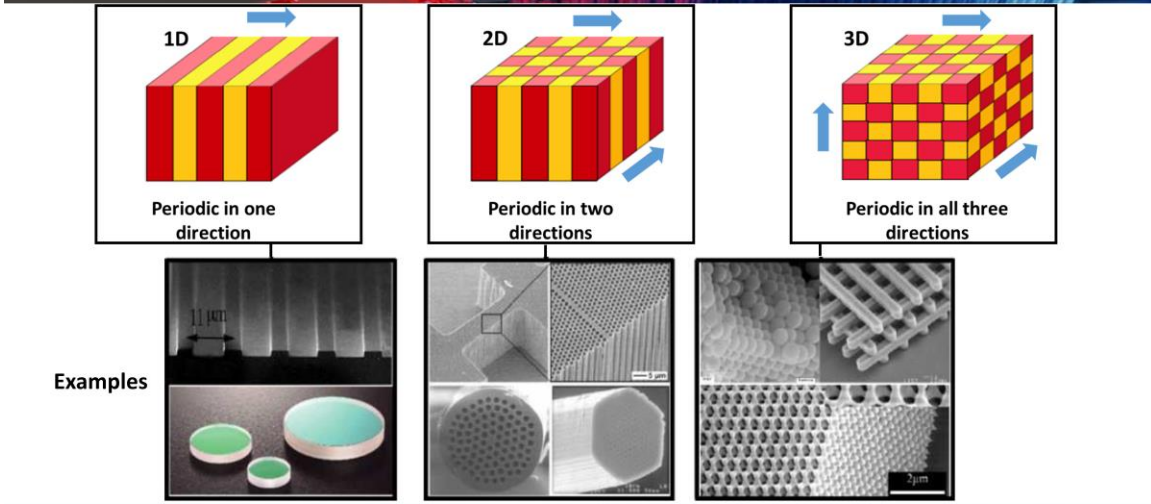
- The optical analogue of an ordinary crystal: **Three-dimensional (3D) photonic crystal**
- **Three-dimensional photonic crystal:** A dielectric structure that is periodic along three different axes



These are kind of you know different types of photonic crystals. So, to introduce this topic we have already discussed about 1D and 2D photonic crystals. So, if you go for 3D photonic crystals they are basically optical analog of ordinary crystals. Because ordinary crystals also exist in three dimension space.

So three-dimensional photonic crystal is basically a dielectric structure where the refractive index modulation happens in all three axis or all three dimensions. So just to summarize this is what happens in 1D photonic crystal, this is what happens in 2D photonic crystal and this is what happens in 3D photonic crystal that means it is periodic in all three directions. Now let us take some examples of 3D photonic crystals. So if you just for recap if you try to you know look into some examples of 1D photonic crystal Bragg grating okay and dielectric mirrors will immediately come to your mind. Okay, if you think about 2D photonic crystals, okay, the photonic crystal fibers that you see here, okay, and the planar photonic crystal, this kind of things should come to your mind.

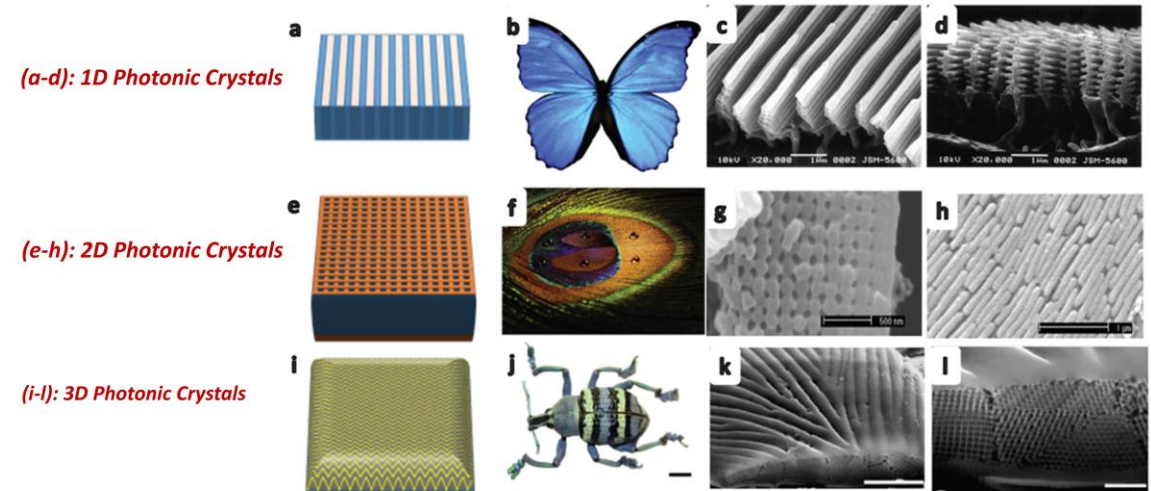
3D Photonic Crystals: Examples



IIT Guwahati | NPTEL | swayam Source: K. Inoue and K. Ohtaka, Photonic Crystals: Physics, Fabrication, and Applications, Vol. 94, Springer Science & Business Media, 2004.

And whenever you think of three-dimensional photonic crystal, okay, this kind of opal structure, wood pile structure or inverse opal structure, these things should come into your mind. So, these are all three-dimensional modulation of refractive index. So, let us take some examples of naturally existing examples of 1D, 2D and 3D photonic crystals. So, photonic crystal structures are very commonly found in nature. So, like whenever you see some bright colors coming from some insects or natural elements, all may not be because of their pigmentation.

3D Photonic Crystals: Examples



IIT Guwahati | NPTEL | swayam Source: H. Inan et al., Photonic crystals: emerging biosensors and their promise for point-of-care applications, Chemical Society Reviews, 46(2), pp.366-388, 2017.

they may be strongly reflecting some particular color of light. And if you take example of Morpho butterfly, which is shown here, you can see, if you see these bright colors coming from the wings and if you take the SEM image of the wings, you can see that these are

basically 1D photonic crystal, which are reflecting this particular color. That means this color falls within the band gap of this photonic crystal, so it cannot penetrate. Remaining colors pass through but only this color okay the bluish color actually coming back to your eyes. If you take example of 2D photonic crystal and if you see a peacock feather under SEM you will see that they are basically having 2D photonic crystal kind of arrangement and this is why you can see these bright colors getting reflected from the peacock feather.

Then you can think of this particular insect which also shows this beautiful reflection okay and when you see this under ACM image you can see that the periodicity is basically in all three dimension and that is why this beetle reflects beautiful colors okay and patterns. Right. So this is the schematic, this is an actual natural object that we are seeing and these are basically the SEM images of the samples.



Three-Dimensional Lattices

- Three-dimensional photonic crystals have all the novel properties of one-dimensional and two-dimensional photonic crystals such as :
 - Band gaps
 - Defect modes
 - Surface states
- In two-dimensional photonic crystals, light can be localized at a defect or at a surface.
- ***With a three-dimensional crystal, the additional capability is added to localize light in all three dimensions.***

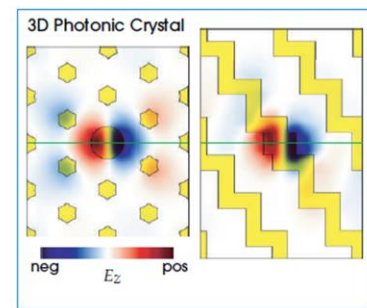


Figure: Light localization in three-dimensional photonic crystals.

Now if you focus only on three-dimensional lattices here. So the three-dimensional photonic crystals all have noble properties.

that we have already seen in the case of 1D and 2D photonic crystals such as band gaps, defect modes and surface states. So this is how you know light localization happens inside a 3D photonic crystal. So if you look at it from you know the top that is you are able to see the 2D pattern okay and then this is from the side you can see that this is where the localization of electric field is taking place right. So, in two dimensional photonic crystals light can be localized at a defect or at a surface and when you take three dimensional photonic crystal the additional capability is added to localize light in all three dimensions.

Three-Dimensional Lattices

- Although there are an infinite number of possible geometries for a three-dimensional photonic crystal, *let's focus on those geometries that promote the existence of photonic band gaps.*
- The two-dimensional crystal with a complete band gap had dielectric “veins” for the TE polarization (in the plane) and dielectric spots for the TM polarization (out of the plane).
- However, the spots were actually long channels running in the z direction, parallel to the TM field.

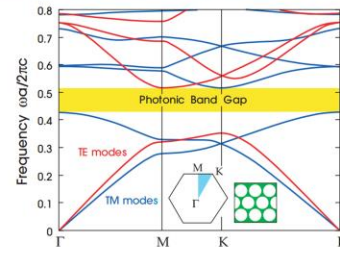
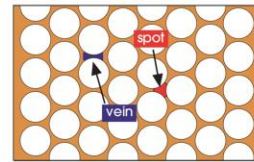


Figure: The photonic band structure for the modes of a triangular array of air columns drilled in a dielectric substrate ($\epsilon = 13$).



So, you can actually have a micro cavity formed ok or something like a resonator cavity formed inside your 3D photonic crystal.

So, although there are an infinite number of possible geometries for three-dimensional photonic crystal, let us first focus on some geometries which promote the existence of the photonic bandgaps. So, if you remember the discussion from two-dimensional photonic crystal which has got a complete bandgap, complete bandgap means the bandgap exists for both the polarization for all the values of the wave factor. right. So, we actually thought of this kind of a structure where you have veins dielectric veins okay connecting these spots okay or major dielectric concentrated regions okay. So, these veins are giving you band gap for TE polarization which is the polarization the electric field is in the plane.

And you can think of an array of dielectric spots, which give you a band gap for TM polarization, which means out of plane electric field vectors, right?

Three-Dimensional Lattices

- So, more generally, a network of dielectric channels running along all the directions needs to be created in which the electric field can point.
- In three dimensions, then, try creating the crystals with arrays of tubes and spheres, analogous to the veins and spots in the two-dimensional lattices or to the bonds and atoms of crystalline atomic lattices.

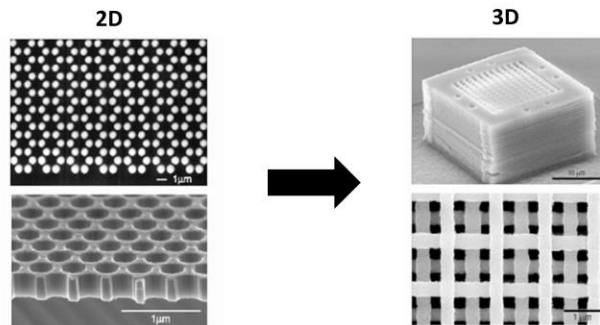


Figure: Scanning Electron Microscopy images of 2D and 3D Photonic Crystals built using lithographic techniques.

So, using this kind of a structure, we saw previously that we are able to get a complete band gap, right? Now what happens in this two-dimensional case, the spots and they actually go along the z direction infinitely, right. So they are basically parallel to the TM field. So this is how you can think of the 2D structure, right. This is the SEM image and this actually goes very large, okay. So generally you can think of a network of dielectric channels which is running along all direction is needed to be created in which electric field can point.

Three-Dimensional Lattices

- It turns out that the choice of the lattice and how it is connected is critical in determining how easily a band gap can be obtained.
- We will investigate several possibilities in this lecture.

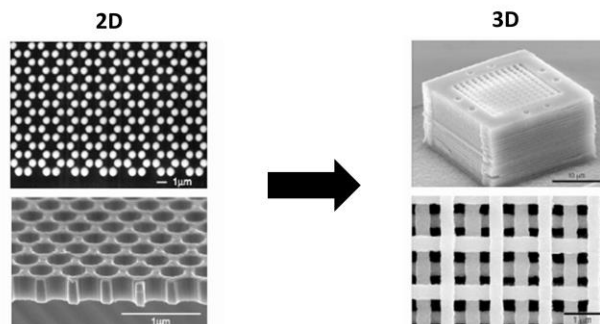


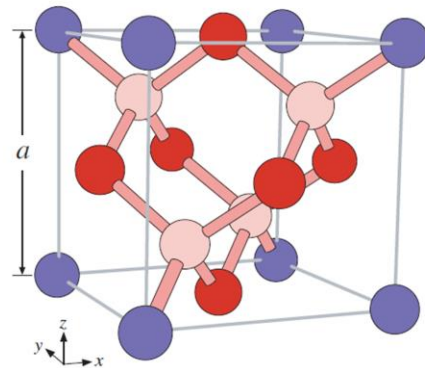
Figure: Scanning Electron Microscopy images of 2D and 3D Photonic Crystals built using lithographic techniques.

So if you think of three dimension okay you can actually try creating crystals with array of tubes and spheres okay which is analogous to the veins and the spots in two dimensional

lattice or these are basically kind of replicating the bonds and atoms of crystalline atomic lattices. So this is how the 2D and 3D photonic crystal looks like and if you look them under SEM okay so this is how the interconnected veins and spots will look like. So, it turns out that the choice of the lattice and how it is connected is very critical in determining how exactly the band gap can be obtained. It means you have the complete control on engineering the band gap in case of these photonic crystals right. So, in this lecture we will basically investigate several possibilities of creating band gap.

Three-Dimensional Lattices

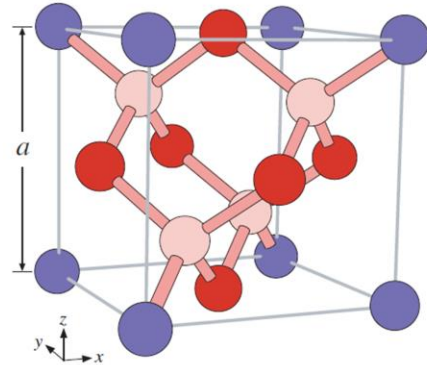
- A schematic representation of several three-dimensional lattices of spheres in a cubic cell is shown.
- The simplest lattice is formed by the blue spheres at the corners of the cube, with primitive lattice vectors \hat{a}_x , \hat{a}_y , and \hat{a}_z .
- This is the **simple cubic** lattice.



So, this is a very common three dimensional lattice Okay so here you can see the simplest one can be considered of this only blue sphere. So this is a cubic lattice and you just consider the blue spheres which are at the corners. So this is basically a simple cubic kind of a lattice right and you can think of the primitive lattice vectors to be $a_x \hat{a}_x$, $a_y \hat{a}_y$, and $a_z \hat{a}_z$. The caps are being placed at the wrong position where a is basically the lattice vector. Now, if you only consider the blue balls they are basically giving you a simple cubic lattice ok.

Three-Dimensional Lattices

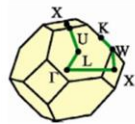
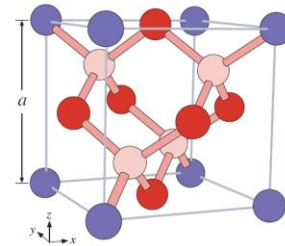
- Ball-and-stick (“atomic”) representation of several three-dimensional lattices in a cubic supercell, with a lattice constant a .
- The blue balls alone form a simple cubic lattice.
- Adding the dark red balls produces a face-centered cubic (fcc) lattice.
- Adding the pink balls as well produces a diamond lattice, with stick “bonds” (four bonds per ball).



However, if you consider blue balls as well as the red balls. So, the red balls are basically at the centre of the face ok. So, you start seeing a FCC lattice right. So, you have this blue balls at the corners and then you have this red balls at the centre of the face. So, this is basically FCC lattice and then if you take you know one pink ball that is equidistant from this red balls and it is connected to you know four balls something like one blue balls and other three red balls.

Three-Dimensional Lattices

- If the dark red spheres are added at the centers of the faces, a **face-centered cubic (or fcc)** lattice is obtained.
- The fcc lattice vectors are $(\hat{x} + \hat{y})a/2$, $(\hat{y} + \hat{z})a/2$, and $(\hat{x} + \hat{z})a/2$.
- For the fcc lattice, the smallest repeating unit (the **primitive cell**) is not the cubic cell shown in figure.
- Rather, the primitive cell is a rhombohedron (with volume $a^3/4$) whose edges are the three lattice vectors.



The cubic cell contains four copies of this primitive cell, and is an example of a supercell.

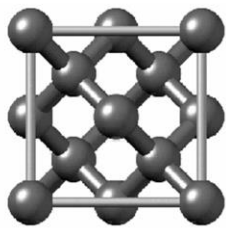
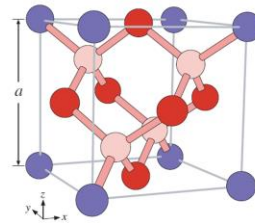
So, this is basically creating a diamond lattice. So, this we have already discussed. So, if you

only consider the dark red spheres, we are basically getting the FCC lattice and for FCC lattice, the lattice vectors are like halfway. So, it is like $(x_{cap} + y_{cap})a/2$ and then you have $(y_{cap} + z_{cap})a/2$ and then you have $(x_{cap} + z_{cap})a/2$, that is correct. So, in the case of you know FCC we have also understood that the primitive cell is basically a rhombohedron ok.

This we have already seen in the previous lectures and this has a typical volume of $a^{3/4}$ ok. So, the edges of this rhombohedron are basically the three lattice vectors and here you actually can see the irreducible Brillouin zone being banked and the important points of symmetry are also mentioned like X, U, l, gamma, X, W, K okay these are the important points of symmetry. Now the cubic cell that contains four species of this primitive cell okay. So this one if you think of this big cell the cubic cell actually contains four such cells okay and this can be an example of a supercell. So you can actually repeat this also to create the abscessy lattice but ideally all the information lives inside the Brillouin zone and also the only independent information can be found inside the irreducible Brillouin zone.

Three-Dimensional Lattices

- Finally, if the pink spheres are added, which represent another fcc lattice that is shifted by $(a/4, a/4, a/4)$ relative to the blue spheres, then a **diamond lattice** is obtained.
- The periodicity in this case is the same as for the fcc lattice, but there are two "atoms" per rhombohedral primitive cell.



Diamond lattice

- In an atomic diamond lattice, the spheres would be carbon atoms, with each atom bonding to its four nearest neighbors, as illustrated.

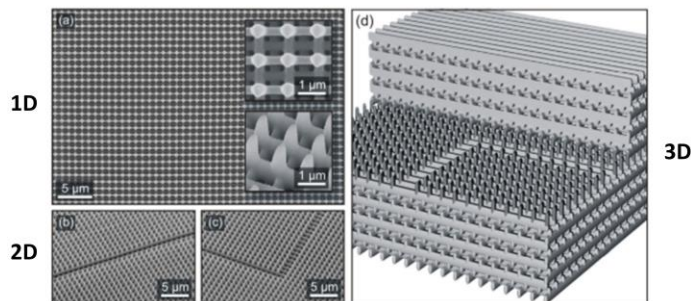
So, for computation purpose if you only consider the irreducible Brillouin zone you can get all the information about the band gap. if you want to spare more you know if you do not want to find out the irreducible Brillouin zone and you have computational resources you go with the Brillouin zone and then if you are too lazy to find the Brillouin zone also you can go with the simple you know primitive cell which is this cubic cell that will also recreate the lattice but then you can imagine the amount of computation you will be requiring to calculate all the possible you know the band gap band structure for this particular cell. So, coming back when you are adding to the pink spheres, when you are going towards the diamond lattice from FCC lattice, you are adding this pink spheres. So, what is happening? It

is basically another FCC lattice which is basically shifted by $a/4$, $a/4$ and $a/4$, okay, relative to the blue spheres. And this is how the diamond lattice is obtained and you can see in this animation how the diamond lattice looks like.

So, this one is at FCC and there is something in the middle of it. So, that is why it is $a/4$, $a/4$, $a/4$, okay. So, the periodicity in this case is same as that for the FCC lattice, okay, just that you will be having two atoms per, okay, rhombohedral primitive cell whereas in case of FCC lattice we will just have one atom inside that right. So sorry so in an atomic diamond lattice the spheres would be simply carbon atoms okay and where each atom is basically bonding to four of its neighbors okay. So why we are studying all these things because this kind of 3D lattices which exist in nature will give us ideas how we can actually place our veins and spots so that we can create the periodicity in three dimension.

Three-Dimensional Lattices

- Returning to the dielectric case, these bonds can be imagined to be dielectric veins.
- They provide the diamond lattice with the requisite channels along which the electric field lines can run.
- *In fact, we shall see that all known photonic crystals with large band gaps (15% or larger with a dielectric contrast of 13 to 1) are closely related to the diamond structure.*



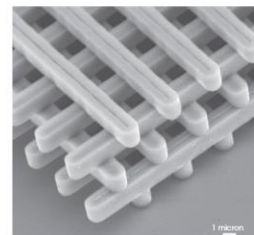
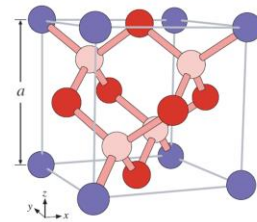
Right. So if you return to our dielectric case, these bonds can be imagined to be the dielectric veins, okay? And they provide the diamond lattice with the requisite channel along the electric field lines can run through those particular veins. So we'll see that all known photonic crystals with large bandgap something like you know 15 percent okay or larger with dielectric contrast of say 13 is to 1 are closely related to the diamond structure. So, here is an example of a different photonic crystal heterostructure okay which can actually help you imagine how a 3D you know structure might look like. So, once again for comparison purpose we are also showing the 1D this is 1D this is ok this is there is a mistake here I think this is not 1D ok. So, returning to the dielectric case this bonds can be imagined to be the dielectric veins and this dielectric veins provide the diamond lattice with

the requisite channel for the electric field lines okay.

So, the electric field lines can run through this dielectric veins and we will see that all the know all of the known photonic crystals with large band gap something like you know 15 percent of larger for dielectric contrast of 13 is to 1. they basically are closely related to the diamond structure. It means diamond structure is a very popular or commonly used structure to obtain 3D photonic bandgaps. So, here is an example of how this structure might look like. So, you need you know periodic modulation of dielectric constant so you need to drill holes in such a way that you are only left with veins and spots veins and spots okay along all three dimension.

Dielectric Contrast of 3D Photonic Crystals

- Consider a photonic crystal composed of only two different substances.
- Let's examine two basic topologies, differing in whether the "atoms" and "bonds" are composed of the high- ϵ material or the low- ϵ material.
- *Note that the ratio of the two dielectric constants that matters most, not the individual values.*



So now we will focus on the dielectric contrast of 3D photonic crystals. So consider a photonic crystal of only two different substances And let us examine two basic topologies differing in whether you know the atoms and bonds are composed of high permittivity material or low permittivity material okay. So, here is an example. So, the ratio of the two dielectric constants that matters most and not the individual values. So that is what you need to keep in mind that we are not interested more on the individual values of the dielectric constant rather we require really a good contrast between the two okay.

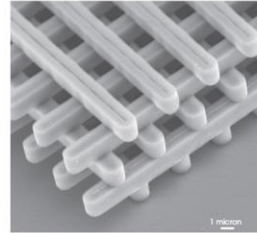
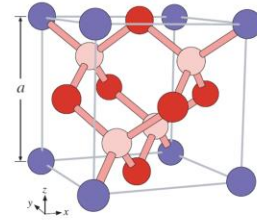
Dielectric Contrast of 3D Photonic Crystals

- Scaling the entire dielectric function by some constant factor:
 $\epsilon(\mathbf{r}) \rightarrow \epsilon(\mathbf{r})/s^2$

results in a trivial rescaling of the band structure, $\omega \rightarrow s\omega$.

- We define the **dielectric contrast** as the ratio of the dielectric constants of the high- ϵ and low- ϵ materials:

$$\text{Dielectric contrast} = \epsilon_{\text{high}}/\epsilon_{\text{low}}$$



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Source: J. D. Joannopoulos et al., "Photonic Crystals: Molding the Flow of Light", Princeton Univ. Press, 2008.

So usually the lower index is considered to be air and then the upper one can be silicon or something like that or even larger like epsilon equals 13. And then you can scale the entire dielectric function by some constant. So $\epsilon(\mathbf{r})$ can be scaled as $\rightarrow \epsilon(\mathbf{r})/s^2$ and this will result in a trivial scaling of the bench structure where you can replace $\omega \rightarrow s\omega$. So, let us define the dielectric contrast as the ratio of the dielectric constants of the high and the low permittivity material. So, this is how you can define what is dielectric contrast.

Band Gaps of 3D Photonic Crystals

- Band gaps tend to appear in structures with a high dielectric contrast.
- The more significant the scattering of light, the more likely a gap will open up.
- One might wonder whether *any* dielectric lattice has a photonic band gap for sufficiently high dielectric contrast.
- This is, in fact, the case for most two-dimensional crystals, at least for one polarization.

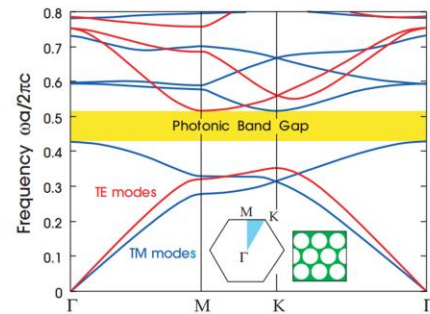


Figure: The photonic band structure for the modes of a triangular (two-dimensional) array of air columns drilled in a dielectric substrate ($\epsilon = 13$).

Why it is important because larger the contrast we have seen that wider is the band gap and that is good for engineering on the band gap. So, now let us look into band gaps of 3D photonic crystals. So, band gaps appear tend to appear in structures with high dielectric contrast as I mentioned before. The more significant the scattering of light the more likely a gap will open up and one might wonder whether any dielectric lattice has a photonic band gap for sufficiently high dielectric contrast. And this is, in fact, the case for most two-dimensional crystals, at least for one polarization.

Band Gaps of 3D Photonic Crystals

- For three-dimensional crystals, complete photonic band gaps are rarer.
- The gap must smother the entire three-dimensional Brillouin zone, not just any one plane or line.
- For example, in figure, we show the band structure for a face-centered cubic (fcc) lattice of close-packed (tangent) high-dielectric spheres ($\epsilon = 13$) in air.
- Although the dielectric contrast is very large, there is no complete photonic band gap.

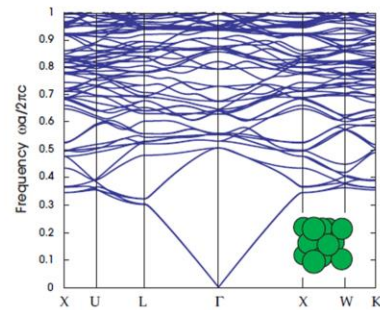


Figure: The photonic band structure for the lowest-frequency electromagnetic modes of a face-centered cubic (fcc) lattice of close-packed dielectric spheres ($\epsilon = 13$) in air (inset).

It may happen that you are not able to excite for both polarization. But yes, with dielectric contrast, more or less along one polarization, you'll be able to see the band gap. Now, you need to do some engineering and try to overlap the two polarizations together something like you can think of this structure it is a two dimensional array or triangular array of air columns which is drilled inside a dielectric substrate of permittivity 13. And there you can see that you are actually getting photonic band gap which is existing for both TE and TM polarization and for the all values of k vector. So we have to aim for something like that.

But when you go to three dimensional lattices complete band gaps are rarer. It is not very usual to find complete band gap in three dimensional crystals and it is much more complicated.

Band Gaps of 3D Photonic Crystals

- *Note the absence of a complete photonic band gap.*
- The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points.

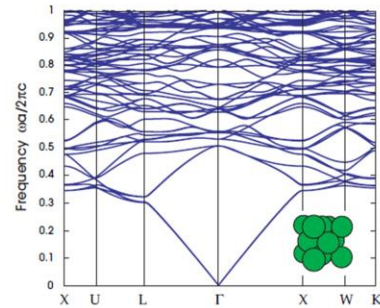
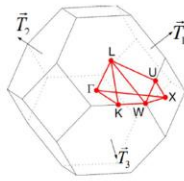


Figure: The photonic band structure for the lowest-frequency electromagnetic modes of a face-centered cubic (fcc) lattice of close-packed dielectric spheres ($\epsilon = 13$) in air (inset).

The gap must smother the entire three-dimensional Brillouin zone, not just any one plane or line and that is why because the Brillouin zone is much larger and complicated in case of 3D crystal so finding a you know complete band gap is challenging so here you can see that if you Consider the bench structure here of an FCC lattice of closely packed high dielectric spheres having permittivity of epsilon 13 and they are all in air but they are closely packed in a FCC lattice and this is what you see. So, although here you can understand that the dielectric contrast is very high, it is 13 is to 1, but can you see any band gap here, photonic band gap? The answer is no. So, for small, small regions you might see some band gap, but you do not have a complete band gap that is for entire, you know, all the directions of the wave vector, okay.

Band Gaps of 3D Photonic Crystals



Face-centered cubic

- K Middle of an edge joining two hexagonal faces
- L Center of a hexagonal face
- U Middle of an edge joining a hexagonal and a square face
- W Corner point
- X Center of a square face

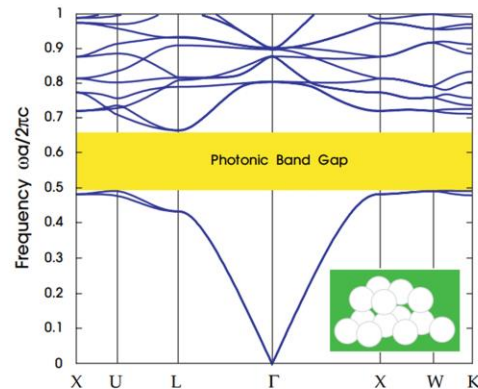


Figure: The photonic band structure for the lowest bands of a diamond lattice of air spheres in a high dielectric ($\epsilon = 13$) material (inset).



Source: J. D. Joannopoulos et al., "Photonic Crystals: Molding the Flow of Light", Princeton Univ. Press, 2008.

So, there is absence of complete photonic band gap. And the wave vector varies across the irreducible Brillouin zone between the leveled high symmetry points, which you have already discussed. So just for a quick recap, so if you have a FCC lattice, so these are your important points. So you can start with X, then you go to U, then you go to l, then you go to gamma, then you go to K. Or you can come back to X and then go to W and K.

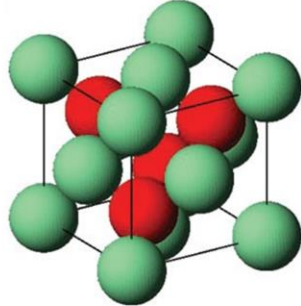
That way also you can traverse or you can go this way. So they have preferred to go like this. So what are these different points? So you can actually see that K is basically the middle of an edge that basically joins two hexagonal faces. What is L? L is the center of an hexagonal face. What is U? U is basically is the middle of an edge which is joining one hexagonal and one square face.

phase. What is W? W is basically a corner point. What is X? X is basically the center of a square phase and these are the primitive reciprocal lattice capital T1, capital T2 and capital T3, right. And this is how when you consider now diamond lattice of air spheres instead of having the solid you know material spheres forming the diamond lattice. If you are able to place air spheres means you need to drill holes at the point of each diamond lattice lattice points you can actually obtain a pretty good complete band gap okay. So, it is pretty wide band gap and it is pretty interesting one.

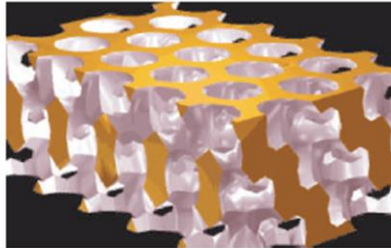
So, this is what you got to do. Here you see the direct structure that is with dielectric spheres of epsilon equals 13 in air could not give you a complete band gap but the inverse structure of it could give you the band gap.

Different types of 3D Photonic Crystals

- A number of three-dimensional crystals have been discovered that yield sizable complete photonic band gaps.



• *Spheres in a diamond lattice*

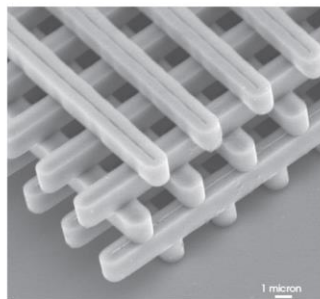


• *Yablonovite*

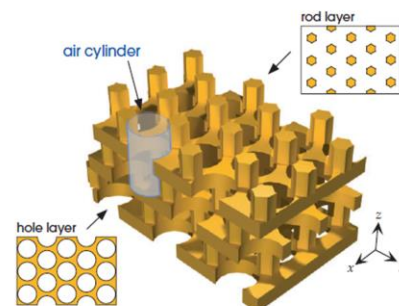
So, now we will look into different types of 3D photonic crystals that can give us you know this complete bandgaps. So, there are a number of three-dimensional crystals that have been discovered that can yield sizeable complete photonic bandgap. So, you can think of this particular structure where in a diamond lattice all the lattice points have got these spheres. Now you can also think of Yablonovite kind of structure which is also a 3D photonic crystal.

Different types of 3D Photonic Crystals

- A number of three-dimensional crystals have been discovered that yield sizable complete photonic band gaps.



• *The woodpile crystal*



• *A stack of two-dimensional crystals*

We will come to this description of Yablonovite in this lecture only after few slides. So these are the two kind of structures that can give us beautiful bandgap. Then you can think of wood pile crystal, wood pile you can think of you know how people pile up you know

wooden logs. So, this is how you can think of the structure okay just that you know this pile and this pile are shifted half the period okay then only you will be able to get that nice band gap okay. And this is a stack of basically two-dimensional crystals.

So you can think of this where you are having air cylinders running through. So as you can understand that 3D photonic crystals are not very easy to fabricate as well.

Different types of 3D Photonic Crystals

- The possibility of three-dimensional photonic band gaps in periodic structures was first suggested by Yablonovitch in 1987, exactly one century after Lord Rayleigh (1887) described one-dimensional band gaps.
- It took three more years, however, before a specific dielectric structure was correctly predicted to have a complete band gap in three dimensions.
- Subsequently, a large number of systems with band gaps have been proposed based on theoretical calculations.
- In many cases, these structures have been fabricated and characterized at wavelengths ranging from the microwave regime to the infrared regime.



Eli Yablonovitch (born 1946) coined the concept of the photonic bandgap; he made the first photonic-bandgap crystal.



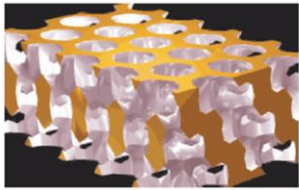
Sajeev John (born 1957) invoked the notion of photon localization and coined the photonic-bandgap concept.

And the possibility of 3D bandgaps, you must have seen this to gentlemen again and again. And again, coming back to them because they have done a great work by talking about 3D photonic bandgap structures in 1987, exactly 100 years or one century after Lord Rayleigh could describe one-dimensional bandgap. So it took 100 years in science to go from 1D to 3D in photonic bandgaps.

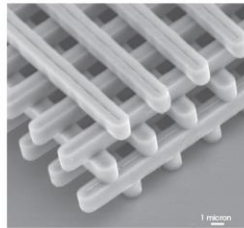
So it took, you know, another three more years before a specific dielectric structure was correctly predicted that could provide a three-dimensional band gap in, you know, it's a complete band gap in 3D. And later on, you know, more number of systems with band gap have been proposed based on theoretical calculations. And this is where theory shows the root for experimentation. So when you find something interesting in theory, you can explore those in experiments. But you should not be trying random experiments hoping that some hidden trial can give you the desired results.

Different types of 3D Photonic Crystals

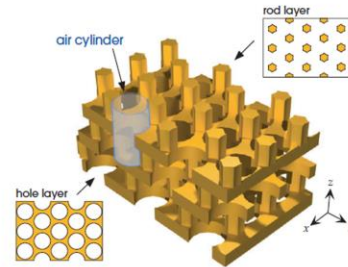
- Many of the successful designs share the same basic topology, and differ mainly in the envisioned fabrication method.
- Let's discuss a few of the most historically important structures, and conclude with a detailed examination of a crystal that is closely related to the two-dimensional systems for a better understanding.



Yablonovite



Woodpile crystal



A stack of two-dimensional crystals



Source: J. D. Joannopoulos et al., "Photonic Crystals: Molding the Flow of Light", Princeton Univ. Press, 2008.

So first, you should do the theory. That is why it is important to understand the theory behind these concepts and how do you calculate this. In a simulation model you are free to choose any parameter and run the simulation again and again that will not add up to your cost but you cannot keep on going and fabricating things and throw it if it doesn't work so that way you will add up to so much of cost for your experimentation and little success. So what they have done they actually fabricated these structures and characterized them at wavelengths ranging from you know microwave to infrared. So they actually first did the experiments in microwave so you know the structure itself was much larger and it was easy to handle. Now, there are currently many successful designs that share basically the same topology, but they differ mainly in the fabrication method. So, you can think of Yablonovite, you can think of wood pile structure and then you can also think of a stack of two-dimensional crystals, right.

So, let us discuss a few of these most historically important structures and conclude with a detailed experimentation of a crystal that is closely related to the two-dimensional systems and that will give us a better understanding of the topic.

Spheres in a diamond lattice

- **K. M. Ho** found the first structure with a complete three-dimensional photonic band gap by considering a diamond lattice of spheres in 1990.
- The structure is similar to the figure, except that the radius of each sphere is large enough to cause the spheres to overlap.

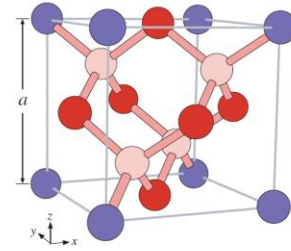


Figure: Ball-and-stick ("atomic") representation of several three-dimensional lattices

- This removes the need for any connecting "bonds."
- It was found that a complete photonic band gap exists whether one embeds dielectric spheres in air or air spheres in a dielectric medium, as long as the sphere radius is chosen appropriately.

So, let us begin with spheres in a diamond lattice. K. M. Ho found the first structure with a complete three-dimensional photonic band gap by considering a diamond lattice of spheres in 1990.

And the structure is very similar to this one except that the radius of each sphere has been considered large enough so that you know the spheres can overlap and you can get something like this okay. So that actually removes the requirement of these bonds. You don't require the connecting bonds. And then it was found that a complete bandgap exists whether one embeds dielectric spheres in air or you consider air sphere in dielectric medium such that you know as long as the sphere radius is chosen arbitrary and that is what we have seen this dielectric structure could not give band gap but when you consider air spheres okay

Spheres in a diamond lattice

- The band structure for a lattice of air spheres within a dielectric medium is shown in the **Figure**.
- To maximize the size of the band gap, the sphere radius r is chosen to be $0.325a$, where a is the lattice constant of the cubic supercell.
- Between the second and third bands, there is a complete gap, with a gap–midgap ratio of 29.6%.

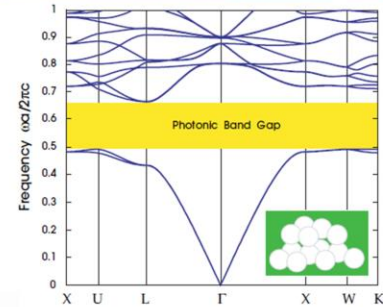
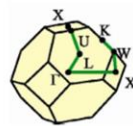


Figure: The photonic band structure for the lowest bands of a diamond lattice of air spheres in a high dielectric ($\epsilon = 1.3$) material (inset).



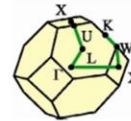
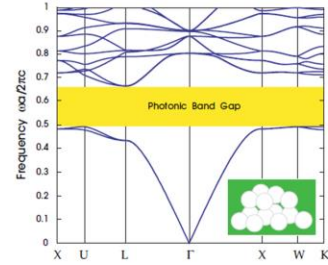
- *A complete photonic band gap is shown in yellow.*

- The wave vector varies across the irreducible Brillouin zone between the labeled high-symmetry points.

in diamond lattice that could give us band gap okay and these points are nothing but this that is why i have repeated this again so it is X U L gamma and then X W K so that is how you can traverse along the boundaries of your irreducible Brillouin zone and you can actually plot this photonic band diagram So what do you see that here are the sphere radius chosen to be $0.325a$ where a is the lattice constant. So this is the optimized value for which you can get the maximum bandgap. And how much is the bandgap? You can see the bandgap does not exist between band 1 and 2, rather it exists between 2 and 3, okay? And that is a complete bandgap and the gap Mid gap frequency ratio is 29.6% which is a pretty pretty good one okay. So this is a complete photonic band gap which is shown in yellow here okay. So remember that in this particular structure the most of the structure is basically air.

Spheres in a diamond lattice

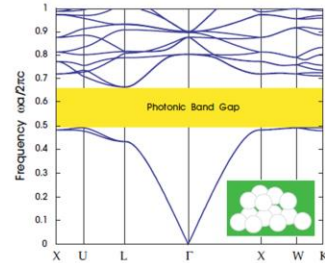
- Most of this structure (81% by volume) is air.
- As noted above, the diameter of the spheres ($0.65a$) is larger than the distance between them ($a\sqrt{3}/4$), causing the air spheres to overlap.
- Both the air and the dielectric regions are connected; there are no isolated spots of either material.
- Let's think of this crystal as two interpenetrating diamond lattices, one of which is composed of connected air spheres, and the other of which is composed of connected dielectric "remnants."



okay so the diameter of the spheres which is considered to be $0.65a$ is basically larger than the distance between them which is $a\sqrt{3}/4$ so what will happen in that case the spheres will overlap and in that case you know both the air and dielectric regions get connected and there will be no isolated spots of either material. So, if you think of this as two interpenetrating diamond lattices, one of which is composed by say the connected air sphere and the other one is basically composed of connected dielectric remnants. So, remnants are basically the remaining parts right. So these remnants which will also follow the pattern of the bonds are basically acting as the channel along which the electric field lines can run and this supports the modes in the two lowest bands.

Spheres in a diamond lattice

- These remnants, which follow the pattern of the “bonds”, are the channels along which the electric field lines can run, for the modes in the two lowest bands.
- However, they are narrow enough that higher bands are forced out, and the corresponding frequency difference produces the photonic band gap.
- Given this fact, one might expect that in three dimensions we could achieve the same property
 - a complete photonic band gap for a small dielectric contrast
 - if the edge of the Brillouin zone had the same magnitude $|\mathbf{k}|$ in all directions, corresponding to a *spherical* Brillouin zone
- However, there is no three-dimensional crystal with a spherical Brillouin zone.



However, when these channels are narrow enough, the higher bands will be forced out and that will basically create the frequency difference and then that can give you the band gap that you are looking for.

So, given this fact one might expect that the three-dimensional structure could achieve the same properties something like you know a complete photonic band gap for a small dielectric contrast and if the edge of the Brillouin zone had same magnitude which is $|\mathbf{k}|$ in all direction then you can actually think of a spherical Brillouin zone okay. However, there is no three-dimensional crystal existing which can give you spherical Brillouin zone. But you can think that you know it is the FCC one is typically close to a spherical one. This is the closest one, right? So generally what you have seen that in 3D crystals, you get polygonal solid, okay, other than simply getting square or hexagonal in two-dimension, right? So in this case, the bandgaps in different direction generally occur at different frequencies. Now, if the dielectric contrast is large, we can arrange for all of these directional band gaps to be wide enough that can overlap and create a mutual band gap.

Spheres in a diamond lattice

- It is generally a polygonal solid, just as it was a square or a hexagon in the two-dimensional examples.
- Thus, the band gaps in different directions generally occur at different frequencies.
- Only if the dielectric contrast is large, we can arrange for all of these directional gaps to be wide enough to create a mutual overlap.
- *What distinguishes the fcc lattice (and the diamond lattice, which shares the same lattice vectors and Brillouin zone) is that the Brillouin zone is nearly spherical.*
- In some sense, it is the most spherical of all possible three-dimensional lattices.
- Equivalently, the spatial period of the fcc lattice is most nearly independent of the spatial direction.
- *This seems to be the key property that makes the fcc and diamond structures the most favorable cases for creating three-dimensional band gaps.*



Source: J. D. Joannopoulos et al., "Photonics Crystals: Molding the Flow of Light", Princeton Univ. Press, 2008.

And that is how you get the complete band gap. So what distinguishes the FCC lattice and diamond lattice, which is also having similar lattice vectors and Brillouin zone, is that for FCC lattice, the brilliant zone is almost spherical okay. So, it is the most spherical of all you can also think of you know the diamond lattice one is that it is the most spherical of all possible 3D lattices. Equivalently the spatial period of the FCC lattice is nearly independent of the spatial So, more or less it is similar in all the directions okay the spatial period. So, this seems to be a very important property that makes you know FCC and diamond lattice both as the most popular cases or favorable cases for creating three dimensional bandgaps.

Yablonovite

- A slab of dielectric is covered by a mask consisting of a triangular array of holes.
- Each hole is drilled three times (right), at an angle of 35.26° away from the normal and spread out 120° on the azimuth.
- This results in a three-dimensional structure whose $(1\bar{1}0)$ cross-section is shown on the left.
- *The dielectric connects the sites of a diamond lattice, shown schematically in yellow.*
- The dielectric veins oriented vertically $[111]$ have greater width than those oriented diagonally $[1\bar{1}\bar{1}]$.

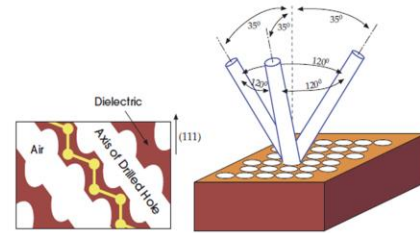


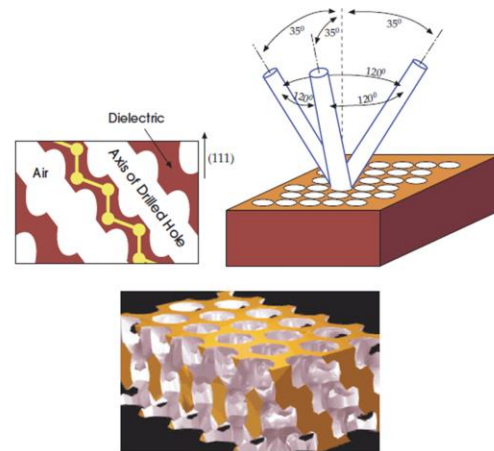
Figure: The method for constructing Yablonovite.

Now, let us look into this particular structure Yablonovite. This is basically named after the scientist who invented it you can actually guess. So, Yablonovich made that particular 3D photonic bandgap crystal. So, in his honor it was named Yablonovite So, let us look into that system more carefully. So, how do you start? You basically start with a slab of dielectric okay which is covered by a mask consisting of triangular array of holes and then each hole is basically drilled three times as you can see here at an angle of 35.26 degrees away from the normal and this three times they are spread across 120 degrees from each other on the azimuth So, when you do that you actually result into this kind of a 3 dimensional structure whose $[1\bar{1}0]$ cross section is shown here.

So, the dielectric connects the sides of a diamond lattice which you can see you know like this that is shown in yellow. And this vertical veins okay or you can see this dielectric veins are oriented along $[1\ 1\ 1]$ direction. They have basically greater width okay than those oriented diagonally that is along $[1\ 1\ \bar{1}]$ direction.

Yablonovite

- *Yablonovite was first fabricated on centimeter scales for measurements of microwave propagation.*
- *Like the diamond lattice of air spheres:
one can think of Yablonovite as two interpenetrating “diamond-like” lattices, one of which is a connected region of dielectric, and the other being a connected air region.*



That way the first structure was created and as I mentioned it was made first for micro propagation and that is the size of the holes everything was much larger they were in centimeter scale and this is how the holes were drilled. So, this is just a cross sectional plane and this is the 3D view of that one.

Yablonovite



- Drilling holes with a radius of $0.234a$ results in a structure with a complete photonic band gap of 19%, as shown in figure.
- Wave vectors are shown for a portion of the irreducible Brillouin zone that includes the edges of the complete gap (yellow).

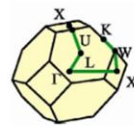
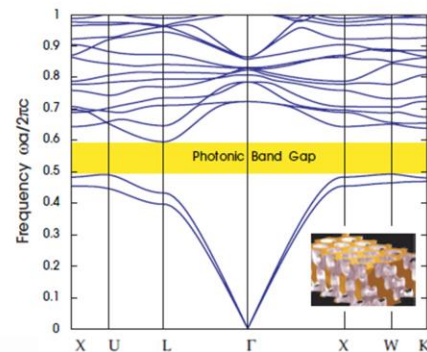


Figure: The photonic band structure for the lowest bands of Yablonovite.

So, what happens here? This act basically creates you know like the diamond lattice of air spheres, ok. So, one can think of Yablonovite as two interpenetrating diamond like lattices, one of which is a connected region of dielectric and the other one is basically a connected air region, ok. So, that mix up gives you this particular beautiful structure. So, when you drill holes of radius $0.234a$ is the lattice period, you can actually get a complete photonic band gap.

So, this has been optimized many, many times and you can actually see the computation gives you a photonic band gap of 19 percent, right. And the wave vectors here basically represent the portion shown for the irreducible Brillouin zone. So, this is how Yablonovite structure could give you around 19 percent you know band gap. So with that we will stop here and we will start discussion about you know three dimensional photonic crystals, more such examples and how we can obtain complete band gap okay in the next lecture. If you have got any query regarding this lecture you can drop an email to me mentioning MOOC and photonic crystal on the subject line. So

Thank You