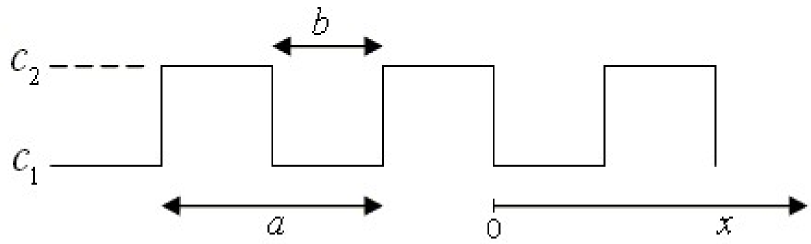
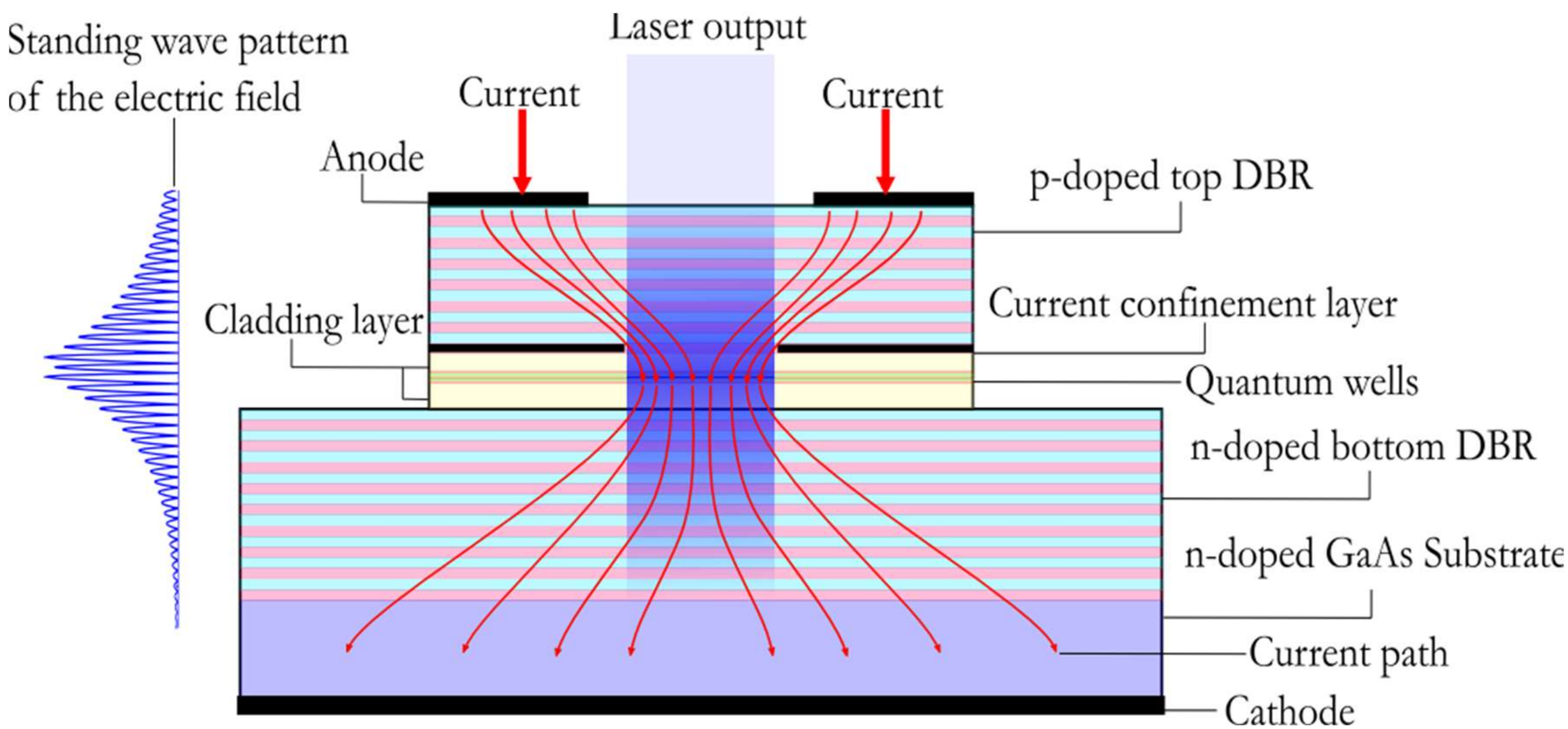
Photon bandstructures

Light in a layered material



The dielectric constant and speed of light are different for the two layers.



Linear differential equations with periodic coefficients

The solutions to a linear differential equation with periodic coefficients,

$$a\frac{d^2\,\xi}{dx^2} + b\frac{d\xi}{dx} + c(x) \quad = d,$$

have the form,

$$\xi = e^{ikx}u_k(x) \qquad \text{where} \qquad u_k(x) = u_k(x+a)$$

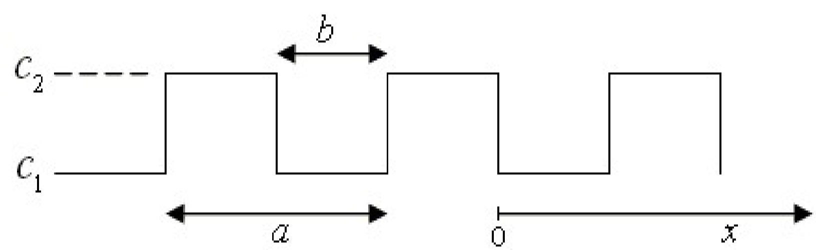
Translational symmetry

The normal modes are eigenfunctions of the translation operator

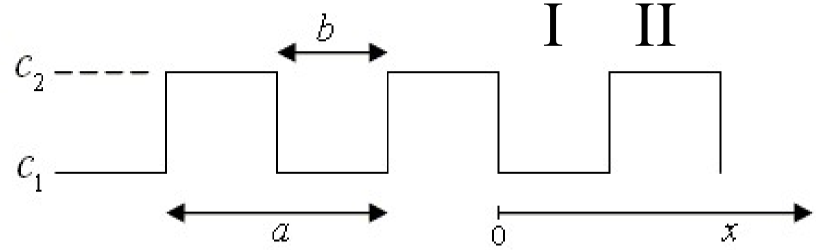
The normal modes have Bloch form.

$$\xi(x) = e^{ikx} u_k(x) \qquad \text{where} \qquad u_k(x) = u_k(x+a)$$

$$T e^{ikx} u_k(x) = e^{ik(x+a)} u_k(x+a) = e^{ika} e^{ikx} u_k(x)$$



Light in a layered material



Hill's equation $$\frac{d^2\xi(x)}{dx^2} = -\frac{\omega^2}{c^2(x)}\xi(x)$$

In region I, the solutions are $\sin(\omega x/c_1)$ and $\cos(\omega x/c_1)$.

In region II, the solutions are $\sin(\omega x/c_2)$ and $\cos(\omega x/c_2)$.

Match the solutions at the boundaries.

Normal modes don't have a clearly defined wavelength.

Solutions in region I and region II

Two linearly independent solutions are specified by the boundary conditions

$$\xi_1(0)=1,\quad \xi_1'(0)=0,\quad \xi_2(0)=0,\quad \xi_2'(0)=1$$

In region I,

$$\xi_1(x)=\cos\left(\frac{\omega x}{c_1}\right),\qquad\qquad \xi_2(x)=\frac{c_1}{\omega}\sin\left(\frac{\omega x}{c_1}\right)$$

In region II,

$$\xi_1(x)=\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(x-b)\right)-\frac{c_2}{c_1}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(x-b)\right),$$

$$\xi_2(x)=\frac{c_1}{\omega}\sin\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(x-b)\right)+\frac{c_2}{\omega}\cos\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(x-b)\right)$$

Translation operator

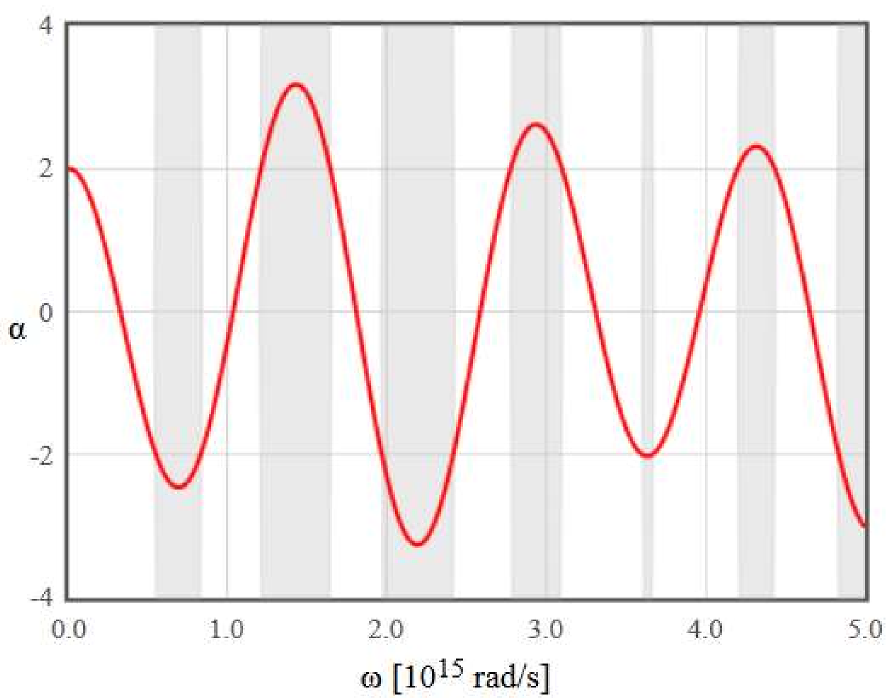
$$\begin{bmatrix} \xi_1(a) \\ \xi_2(a) \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} \xi_1(0) \\ \xi_2(0) \end{bmatrix}$$

The elements of the translation matrix can be determined by evaluating this equation and its derivative at $x = 0$. Diagonalize the translation operator and find its eigenvalues to determine the character of the solutions.

Wave vector

$$k = \frac{1}{a}\tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2} - 1}\right)$$

$$\alpha(\omega) = 2\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(a-b)\right) - \frac{c_1^2 + c_2^2}{c_1 c_2}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(a-b)\right)$$

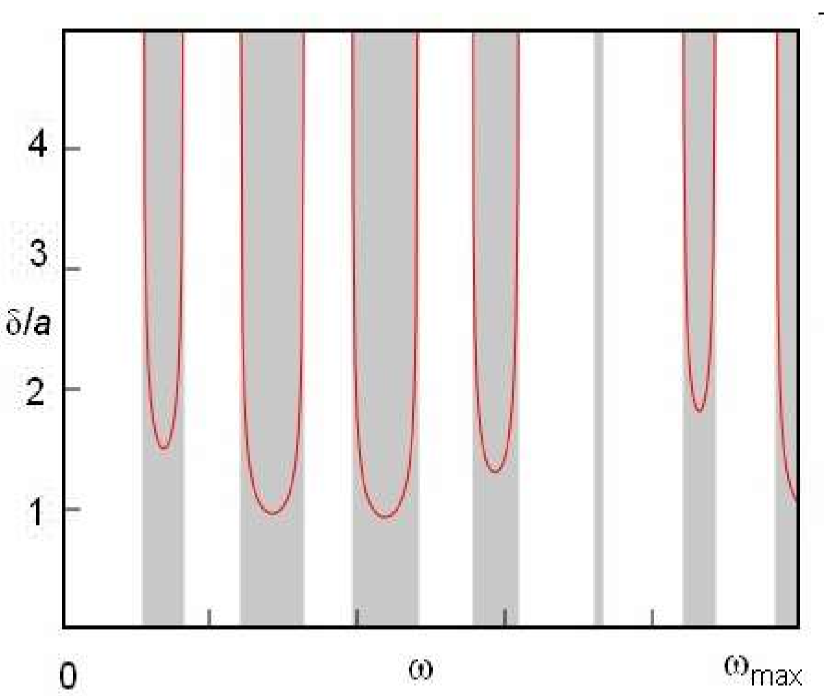


a:	600E-9	[m]
b:	250E-9	[m]
c_1:	2.998E8	[m/s]
c_2:	1E8	[m/s]
ω_{max}:	5E15	[rad/s]

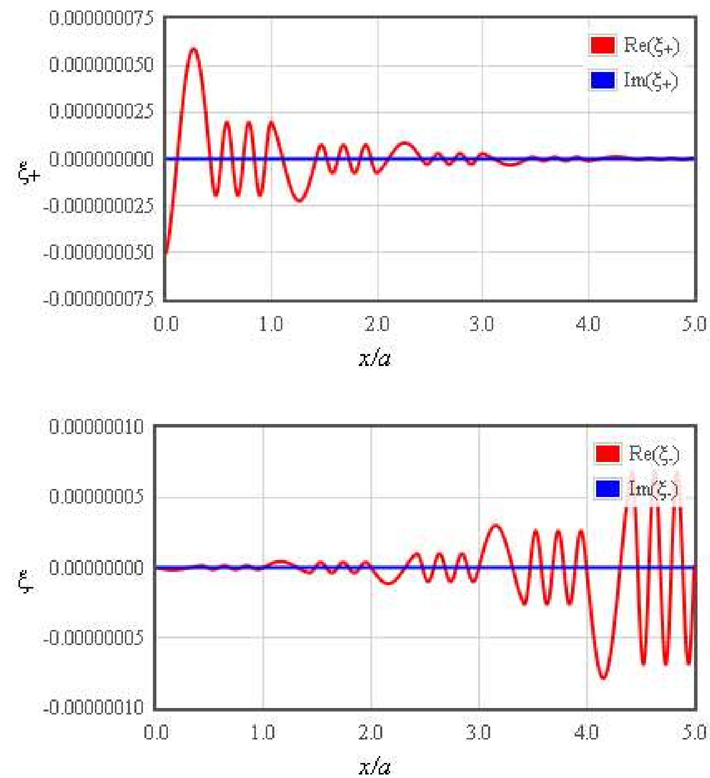
plot

Band gap: exponentially decaying solutions

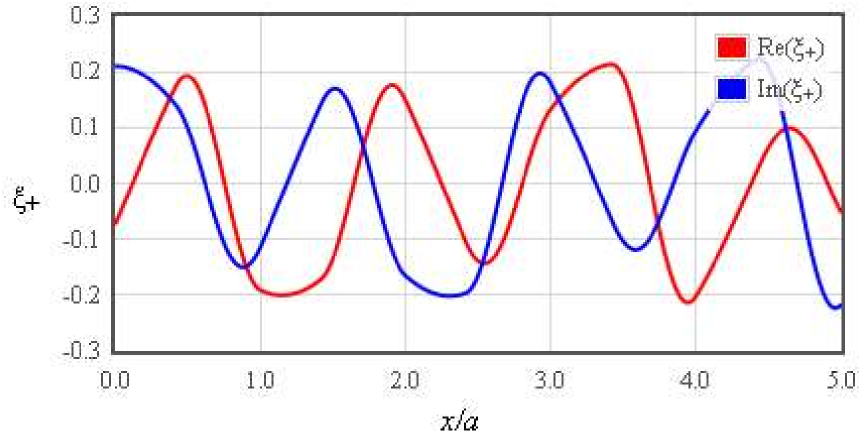
The one solution grows exponentially and the other decays like exp(-x/δ).

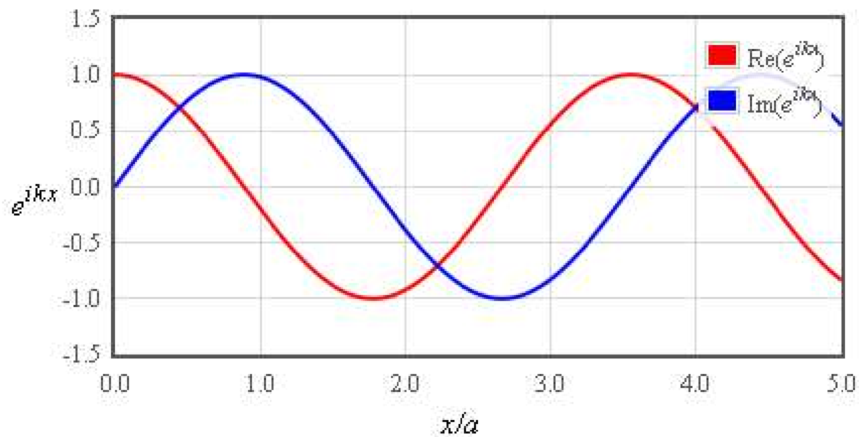


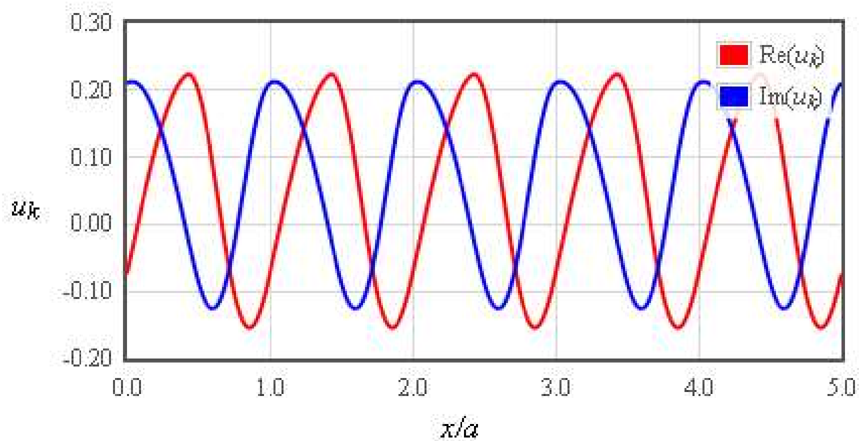
Gray where |α| > 2.



$$\delta = \frac{-a}{\ln\left(\min\left(\lambda_-, \lambda_+\right)\right)}$$







Bloch waves

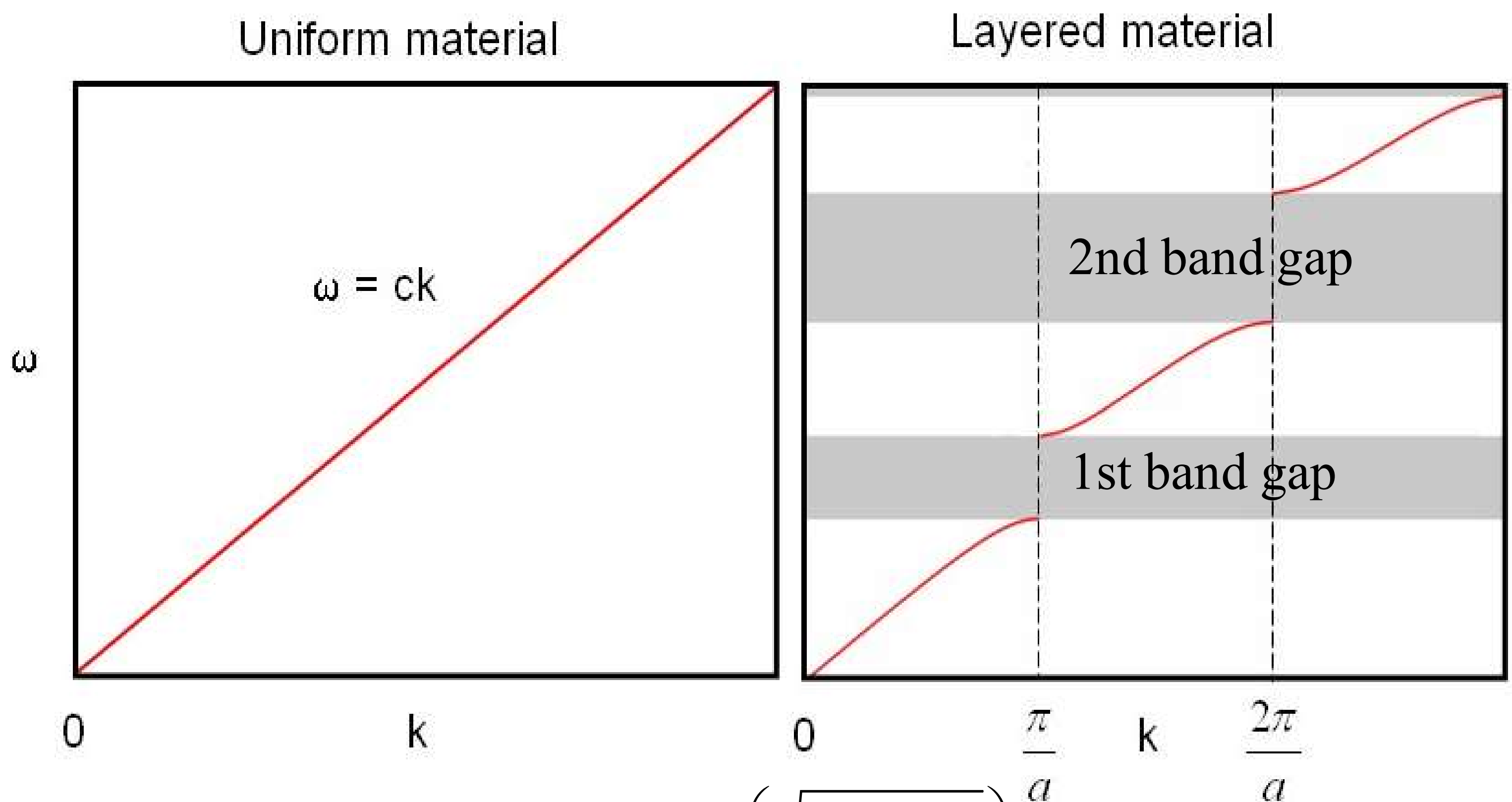
$$\xi = e^{ikx} u_k(x)$$

For periodic boundary conditions $L = Na$, the allowed values of k are exactly those allowed for waves in vacuum.

k labels the eigenfunctions of the translation operator.

$$Te^{ikx} u_k(x) = e^{ik(x+a)} u_k(x+a) = e^{ika} e^{ikx} u_k(x)$$

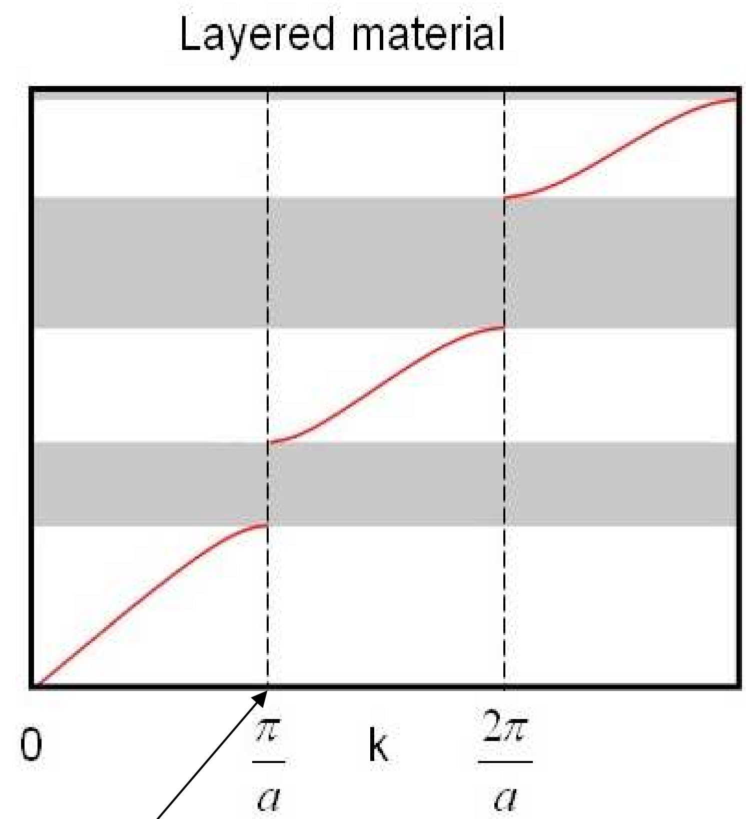
Dispersion relation

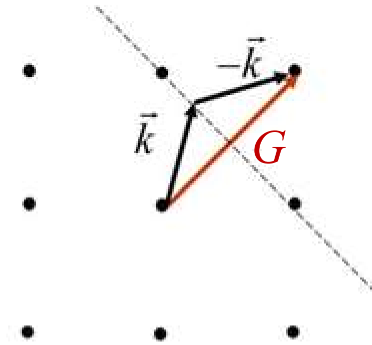


$$k = \frac{1}{a}\tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2}-1}\right)$$

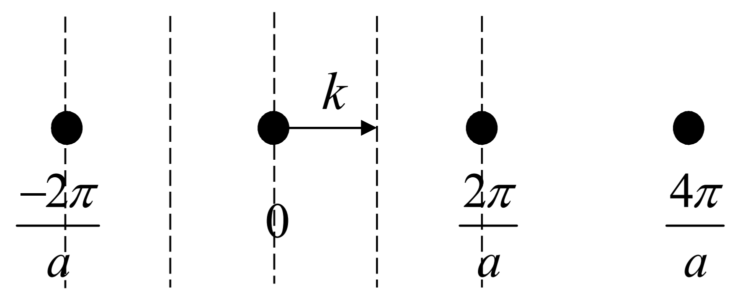
$$\alpha(\omega) = 2\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(a-b)\right) - \frac{c_1^2+c_2^2}{c_1 c_2}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(a-b)\right)$$

Diffraction condition

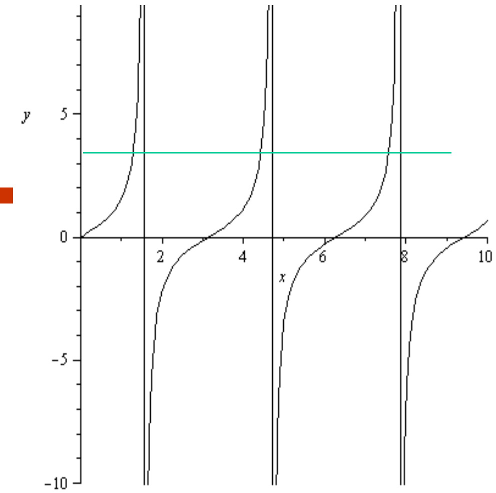




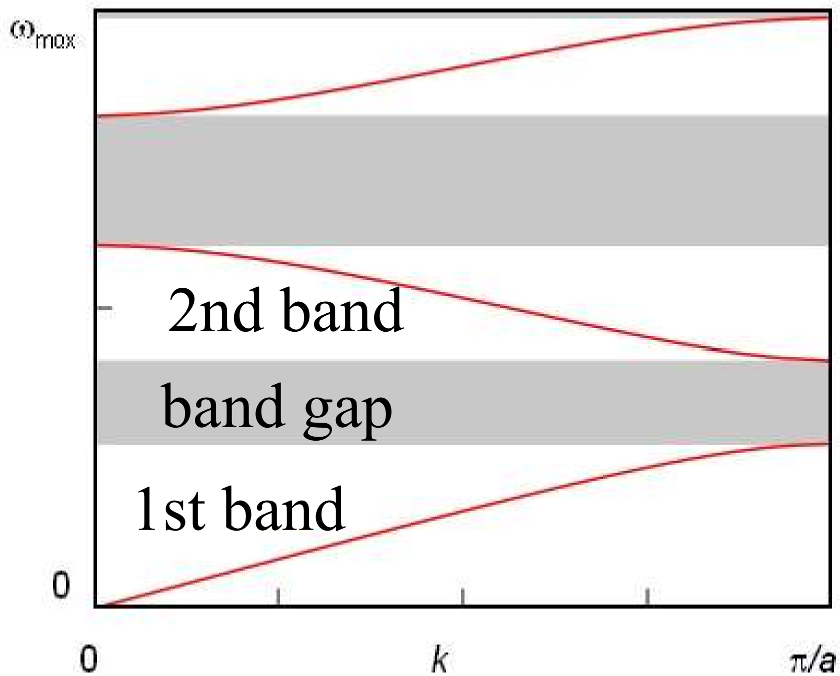
1st Brilluoin zone boundary



Dispersion relation



$$k = \frac{1}{a}\tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2} - 1}\right)$$



$$\tan(ka) = \sqrt{\frac{4}{\alpha^2} - 1}$$

$$e^{ikx}u_k(x) = e^{ikx}\sum_G a_G e^{iGx}$$

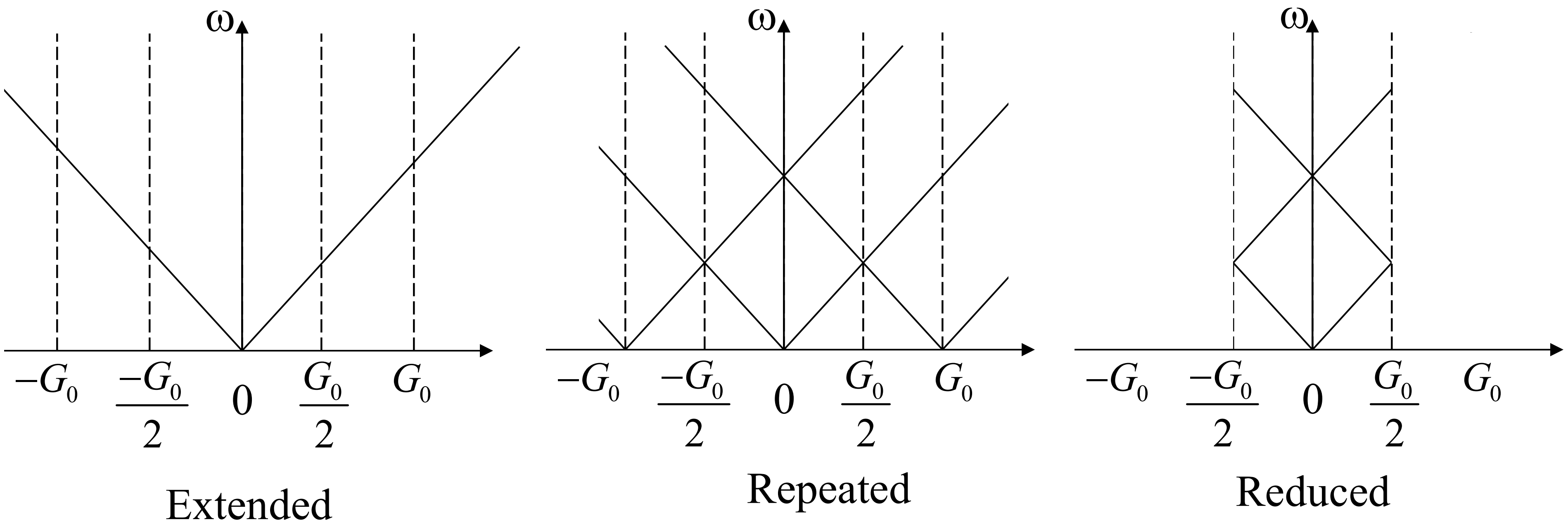
$$k = k' + G'$$

$$e^{ikx}u_k(x) = e^{i(k'+G')x}\sum_G a_G e^{iGx}$$

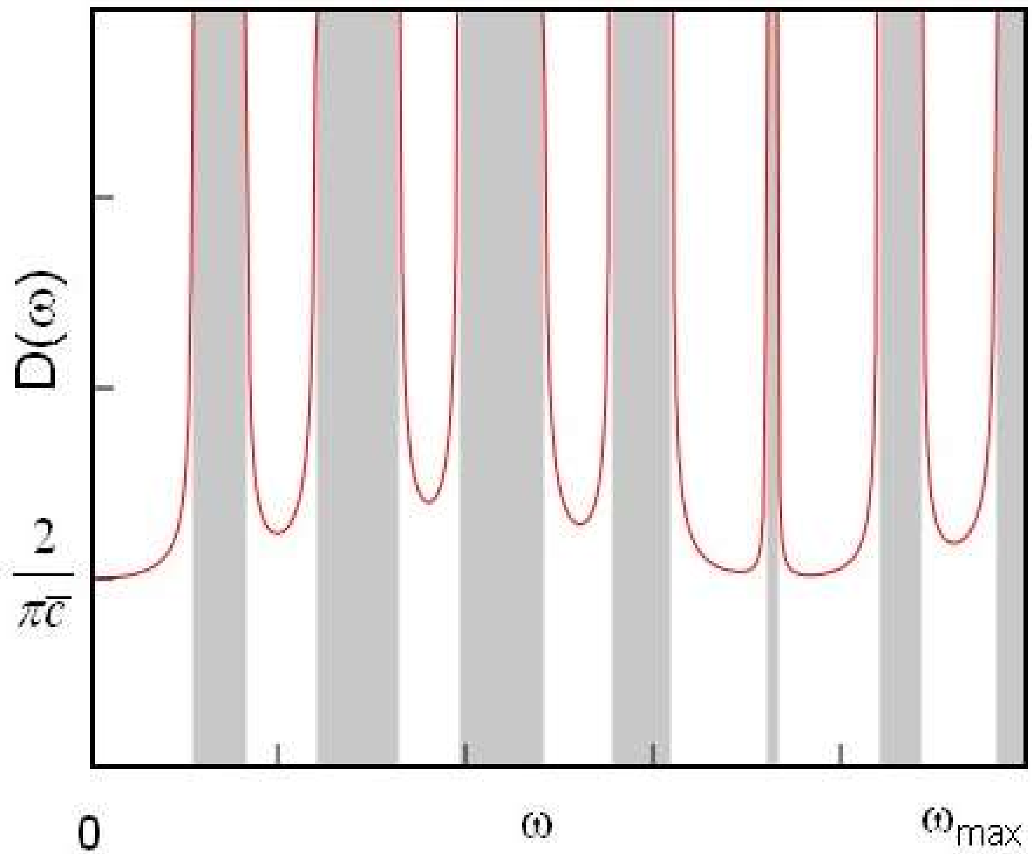
$$e^{ikx}u_k(x) = e^{ik'x}\sum_G a_G e^{i(G+G')x}$$

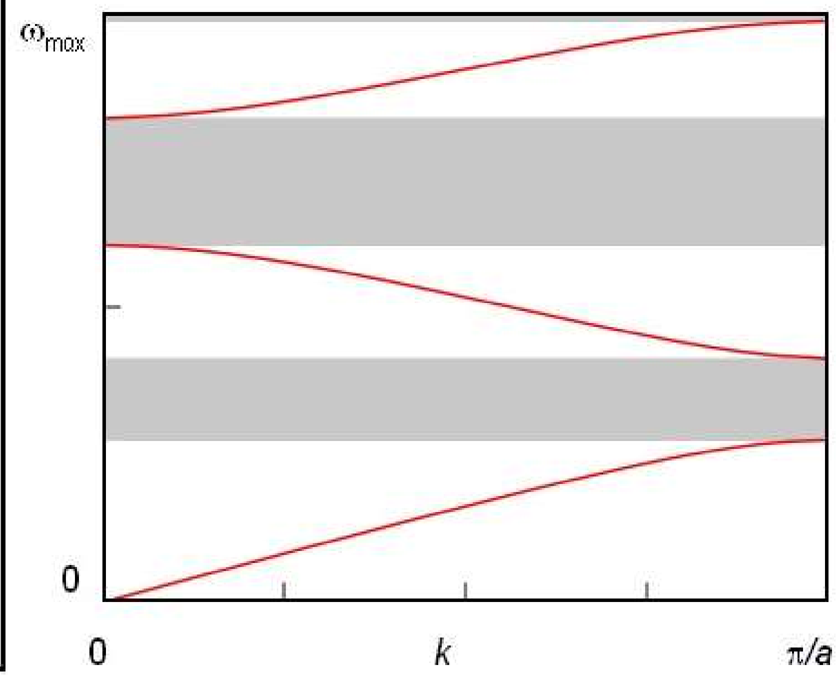
There is only one *k*' in the first Brillouin zone and the convention is to use that one.

Zone schemes



Density of states

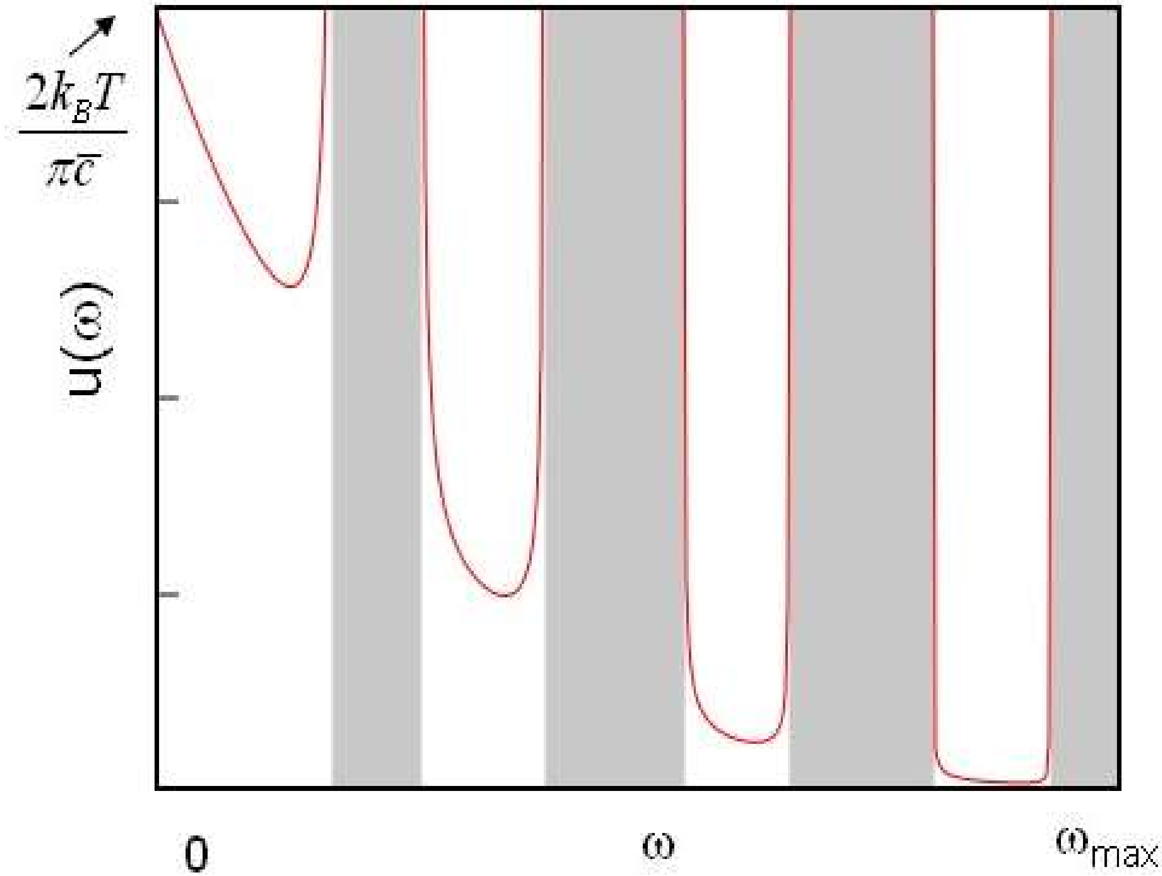




$$D(\omega) = D(k)\frac{dk}{d\omega}$$

The density of states can be determined from the dispersion relation.

Energy spectral density



$$u(\omega) = \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

Analog to the Planck radiation curve.

Thermodynamic quantities

Energy spectral density:

$$u(\omega) = \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

DoS → u(ω)

Internal energy density:

$$u(T) = \int_0^\infty \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega$$

DoS → u(T)

Helmholz free energy density:

$$f(T) = k_B T \int_0^\infty D(\omega) \ln\left(1 - \exp\left(\frac{-\hbar\omega}{k_B T}\right)\right) d\omega$$

DoS → f(T)

Entropy density:

$$s = -\frac{\partial f}{\partial T} = -k_B \int_0^\infty D(\omega)\left(\ln\left(1 - e^{-\hbar\omega/k_B T}\right) + \frac{\hbar\omega}{k_B T\left(1 - e^{\hbar\omega/k_B T}\right)}\right) d\omega$$

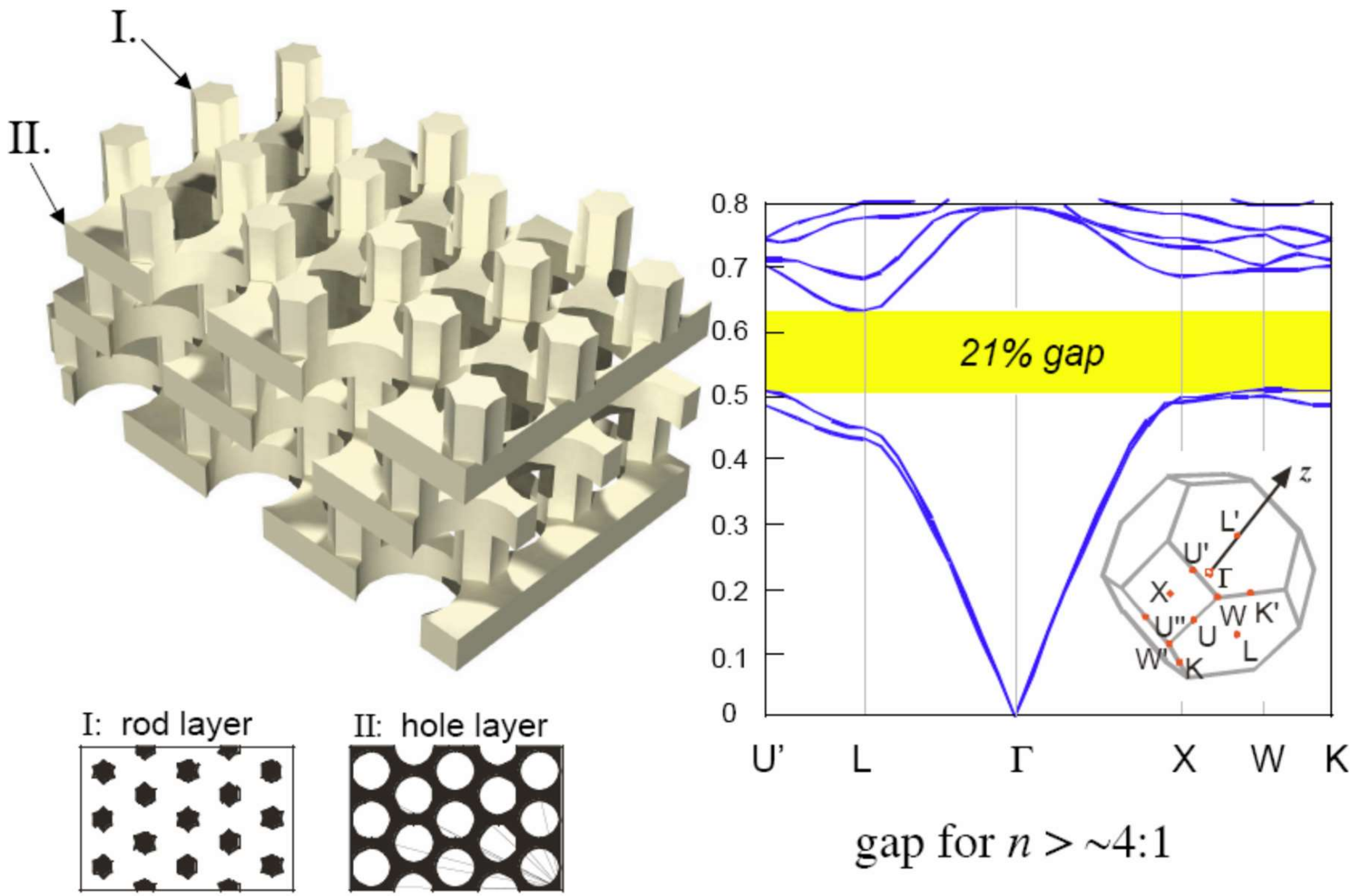
DoS → s(T)

Specific heat:

$$c_v = \int \left(\frac{\hbar\omega}{T}\right)^2 \frac{D(\omega)\exp\left(\frac{\hbar\omega}{k_B T}\right)}{k_B\left(\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1\right)^2} d\omega$$

DoS → cv(T)

3d photonic crystal: complete gap , ε=12:1

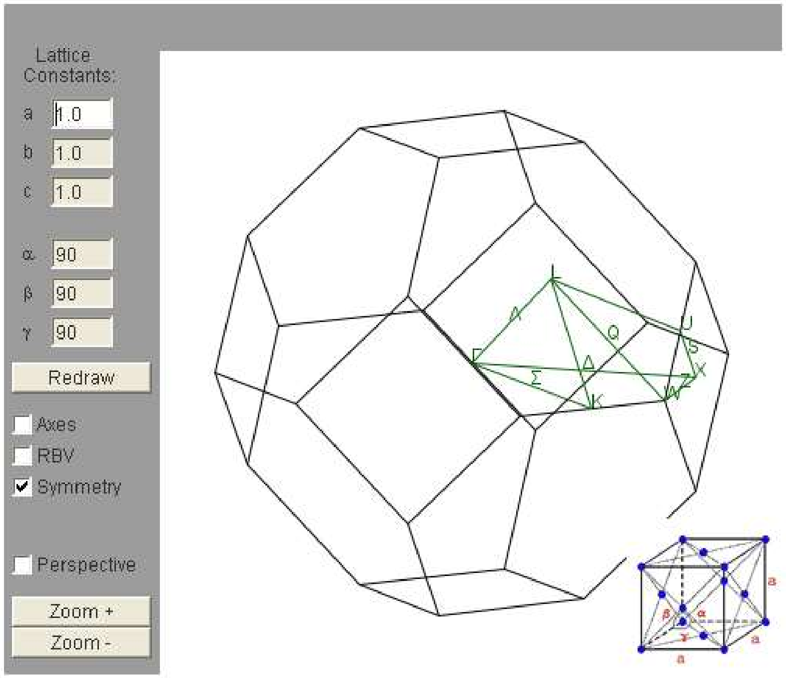


gap for n > ~4:1

[S. G. Johnson *et al.*, *Appl. Phys. Lett.* **77**, 3490 (2000)]

http://ab-initio.mit.edu/photons/tutorial/L1-bloch.pdf

The first Brillouin zone of a face centered cubic lattice



$$\vec{k} = u\vec{b}_1 + v\vec{b}_2 + w\vec{b}_3 \quad : \quad (u,v,w)$$

Symmetry points (u,v,w)	$[k_x,k_y,k_z]$	Point group
Γ: (0,0,0)	[0,0,0]	m3m
X: (0,1/2,1/2)	[0,2π/a,0]	4/mmm
L: (1/2,1/2,1/2)	[π/a,π/a,π/a]	$\bar{3}$m
W: (1/4,3/4,1/2)	[π/a,2π/a,0]	$\bar{4}$2m
U: (1/4,5/8,5/8)	[π/2a,2π/a,π/2a]	mm2
K: (3/8,3/4,3/8)	[3π/2a,3π/2a,0]	mm2

$$\overline{\Gamma L} = \frac{\sqrt{3}\pi}{a}, \quad \overline{\Gamma X} = \frac{2\pi}{a}, \quad \overline{\Gamma W} = \frac{\sqrt{5}\pi}{a}$$

$$\overline{\Gamma K} = \overline{\Gamma U} = \frac{3\pi}{\sqrt{2}a}, \quad \overline{KW} = \overline{XU} = \frac{\pi}{\sqrt{2}a}$$

Symmetry lines	Point group
Δ: $(0,v,v)$ $0 < v < 1/2$	4mm
Λ: (w,w,w) $0 < w < 1/2$	3m
Σ: $(u,2u,u)$ $0 < u < 3/8$	mm2
S: $(2u,1/2+2u,1/2+u)$ $0 < u < 1/8$	mm2
Z: $(u,1/2+u,1/2)$ $0 < u < 1/4$	mm2
Q: $(1/2-u,1/2+u,1/2)$ $0 < u < 1/4$	2

The real space and reciprocal space primitive translation vectors are:

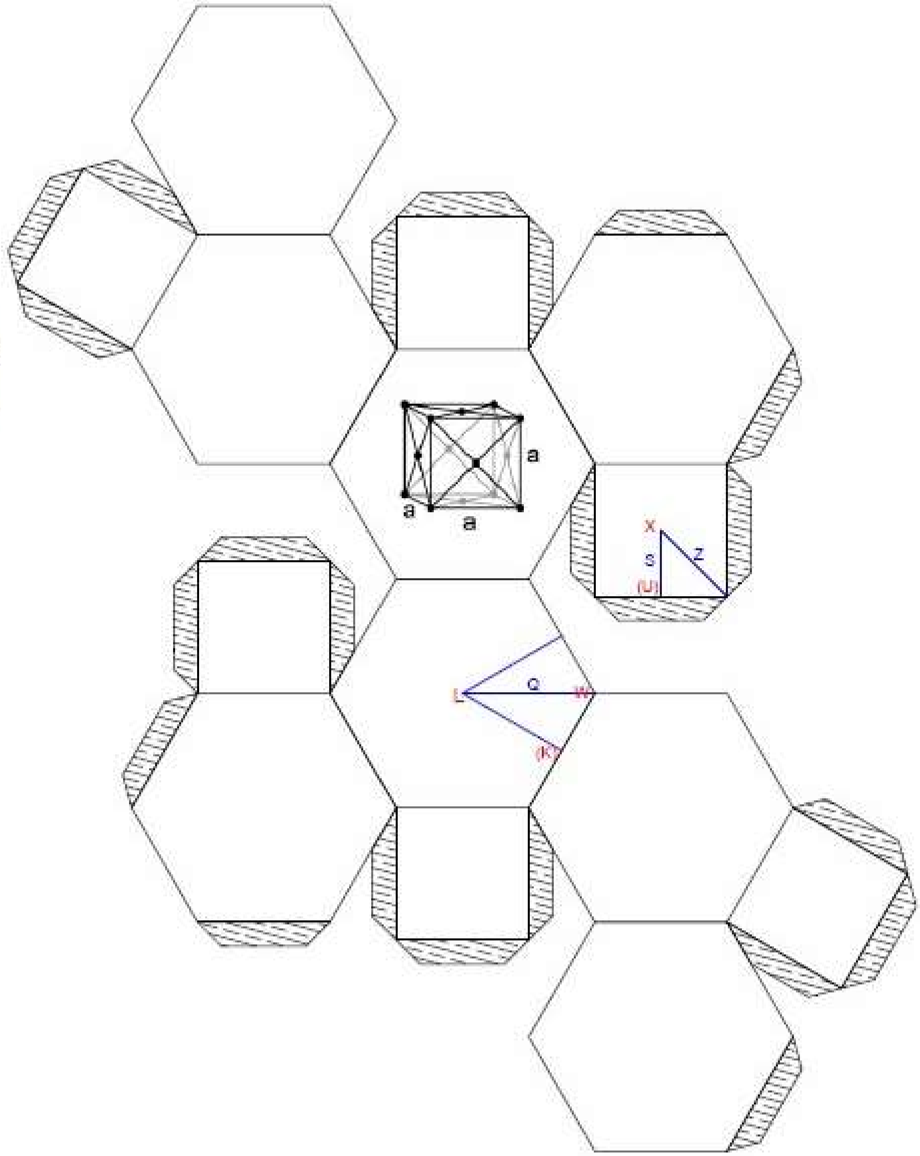
$$\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{z}), \qquad \vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{y}), \qquad \vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{z}),$$

$$\vec{b}_1 = \frac{2\pi}{a}\left(\hat{k}_x - \hat{k}_y + \hat{k}_z\right), \quad \vec{b}_2 = \frac{2\pi}{a}\left(\hat{k}_x + \hat{k}_y - \hat{k}_z\right), \quad \vec{b}_3 = \frac{2\pi}{a}\left(-\hat{k}_x + \hat{k}_y + \hat{k}_z\right)$$

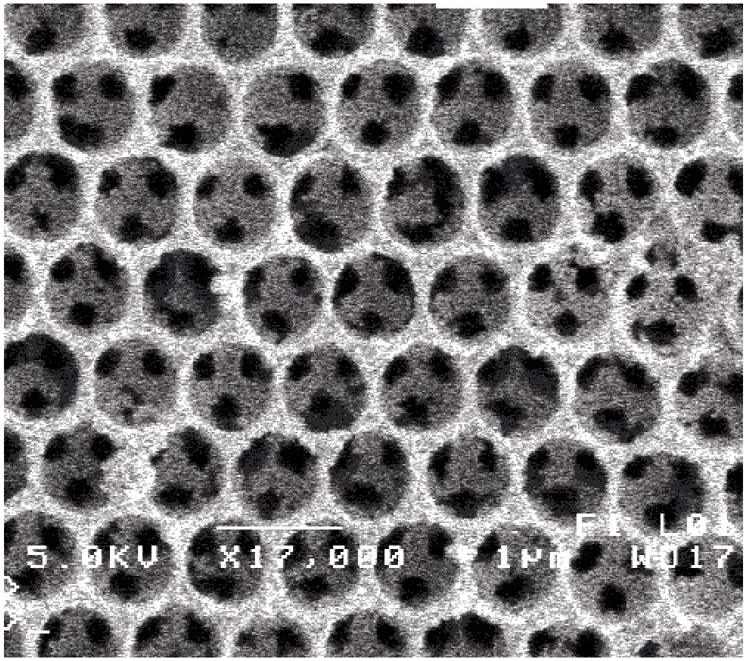
Cut-out patterns for Brillouin zones

Cut-out patterns to make your own models of the Brillouin zones. The symmetry points are red and the symmetry lines are blue.

- simple cubic
- face centered cubic
- body centered cubic
- hexagonal
- tetragonal
- body centered tetragonal
- orthorhombic
- face centered orthorhombic
- body centered orthorhombic
- base centered orthorhombic



Inverse opal photonic crystal



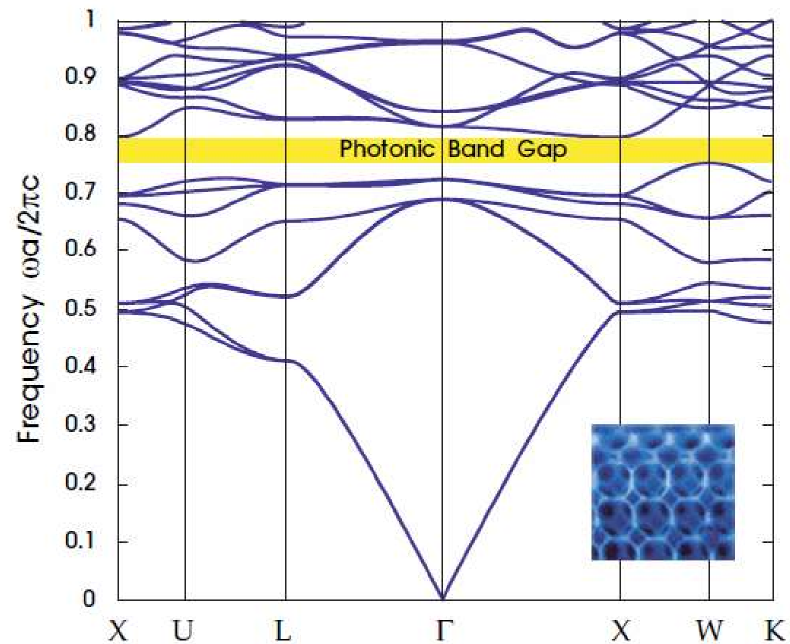
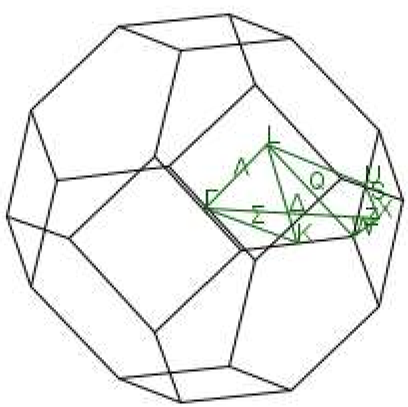


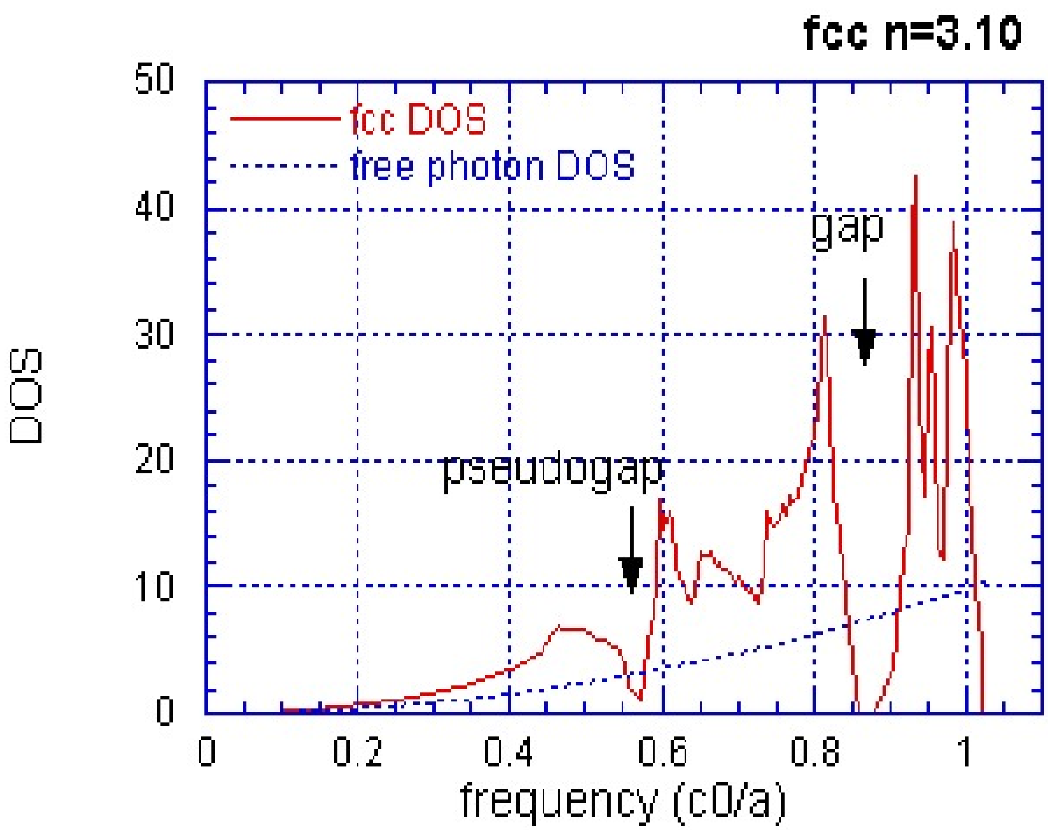
Figure 8: The photonic band structure for the lowest bands of an "inverse opal" structure: a face-centered cubic (fcc) lattice of close-packed air spheres in dielectric ($\varepsilon = 13$). (Inset shows fabricated structure from figure 9.) There is a complete photonic band gap (yellow) between the eighth and ninth bands. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points; see appendix B for a discussion of the Brillouin zone of an fcc lattice.

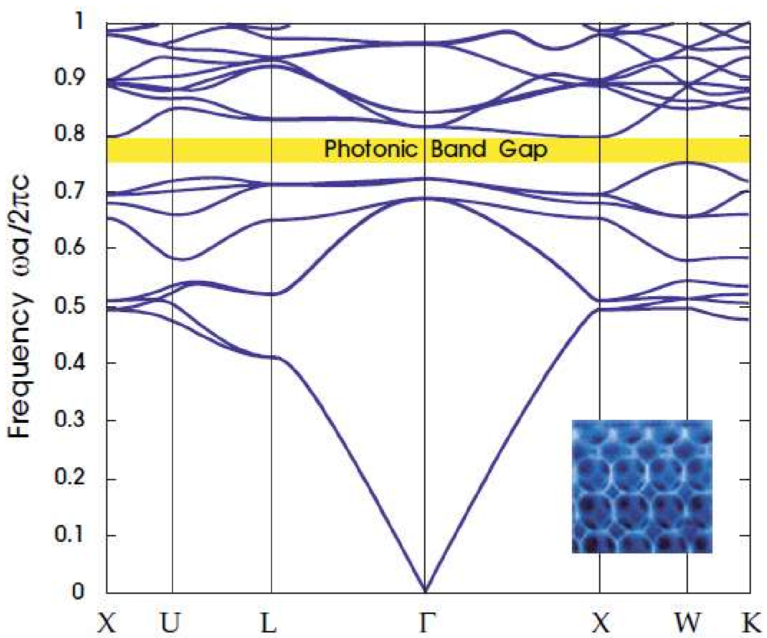


http://ab-initio.mit.edu/book

Photon density of states

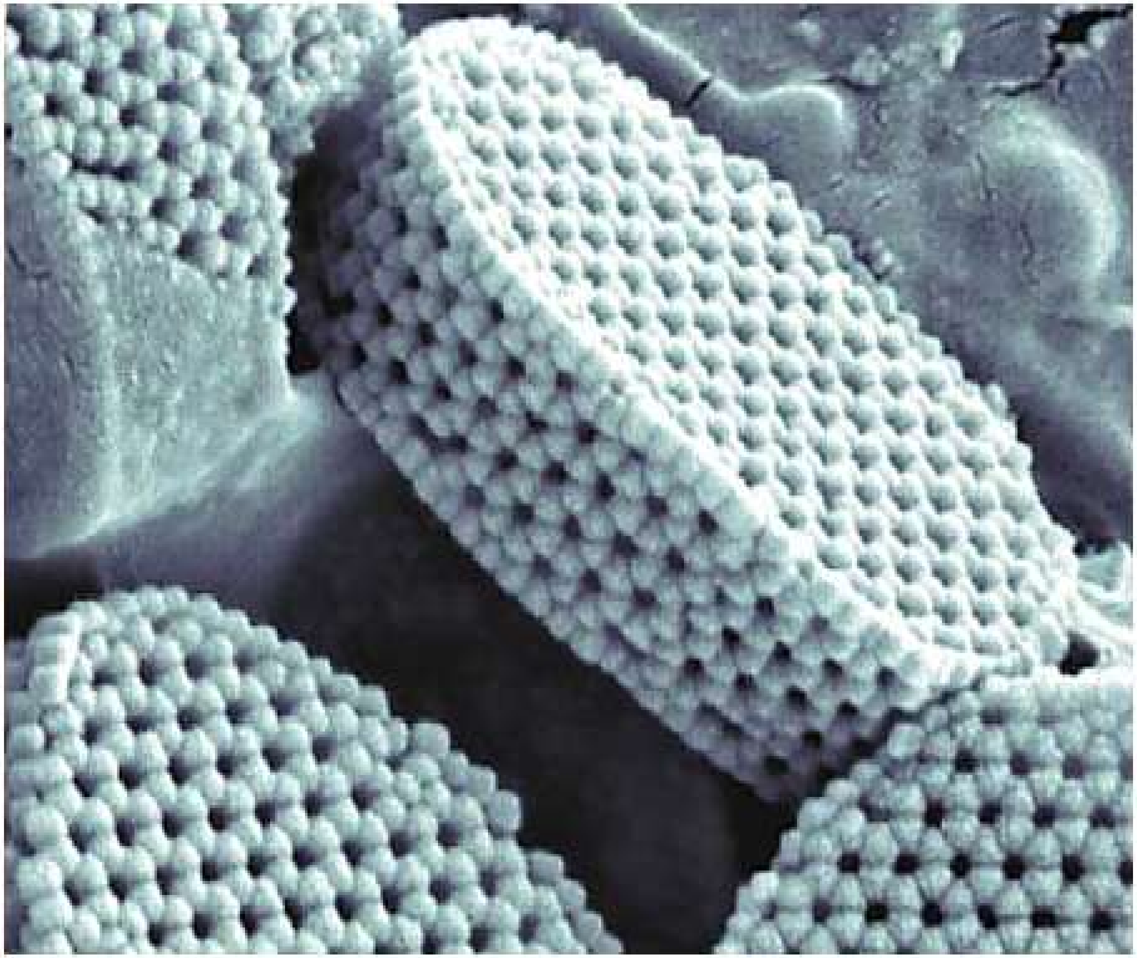
Diffraction causes gaps in the density of modes for *k* vectors near the planes in reciprocal space where diffraction occurs.





photon density of states for voids in an fcc lattice

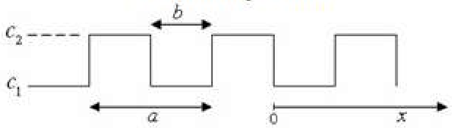
http://www.public.iastate.edu/~cmpexp/groups/PBG/pres_mit_short/sld002.htm



The alga Calyptrolithophora papillifera is encased in a shell of calcite crystals with a two-layer structure (visible on oblique face). Calculations show that this protective covering reflects ultraviolet light. Image Credit: J. Young/Natural History Museum, London

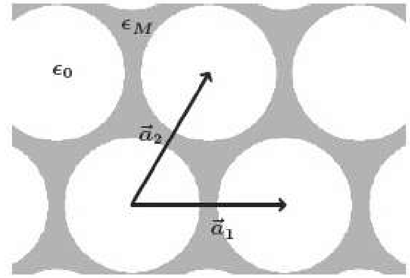
http://www.physicscentral.com/explore/pictures/algae.cfm

1-D Multilayer film

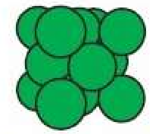


1-D Multilayer film

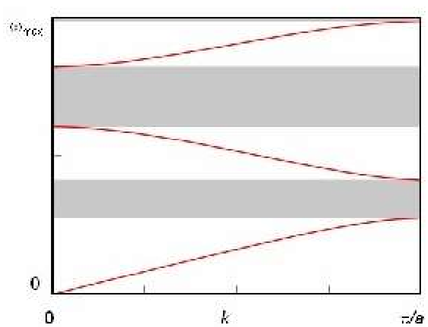
2-D triangular array of air holes



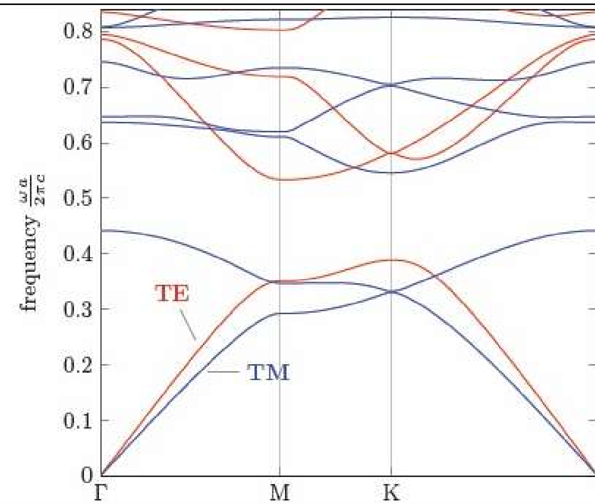
fcc

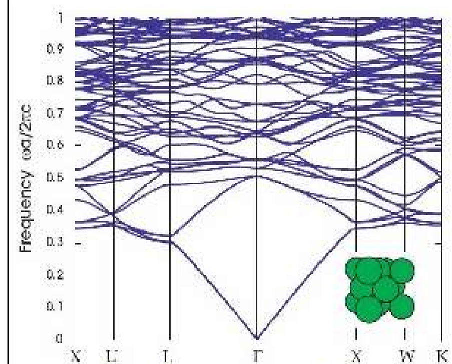


http://ab-initio.mit.edu/book

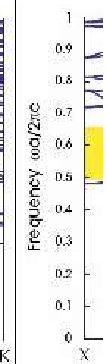


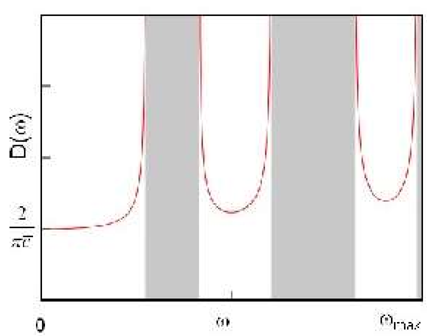
Calculate ω(k)



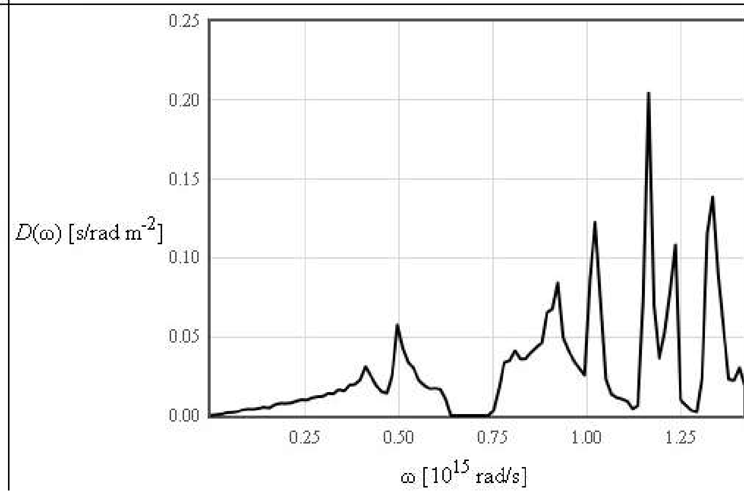


http://ab-initio.mit.edu/book





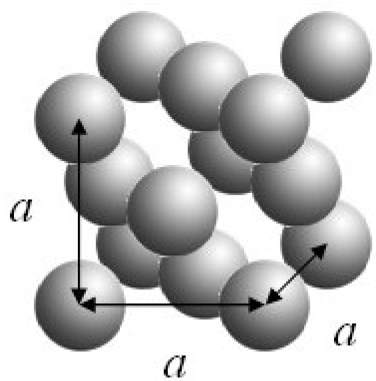
Calculate DoS



http://lampx.tugraz.at/~hadley/ss1/emfield/photonic_crystals/photonic_table.html

Spheres on any 3-D Bravais lattice

$$c(\vec{r})^2 \nabla^2 A_j = \frac{d^2 A_j}{dt^2}$$



opal

$$c(\vec{r})^2 = \sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = c_1^2 + \frac{4\pi\left(c_2^2 - c_1^2\right)}{V} \sum_{\vec{G}} \frac{\sin\left(|G|R\right) - |G|R\cos\left(|G|R\right)}{|G|^3} \exp\left(i\vec{G}\cdot\vec{r}\right)$$

Plane wave method

$$c(\vec{r})^2 \nabla^2 A_j = \frac{d^2 A_j}{dt^2}$$

$$c(\vec{r})^2 = \sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \qquad A_j = \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

$$\sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \sum_{\vec{\kappa}} \left(-\kappa^2\right) A_{\vec{\kappa}} e^{i\left(\vec{\kappa}\cdot\vec{r}-\omega t\right)} = -\omega^2 \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

$$\sum_{\vec{\kappa}} \sum_{\vec{G}} \left(-\kappa^2\right) b_{\vec{G}} A_{\vec{\kappa}} e^{i\left(\vec{G}\cdot\vec{r}+\vec{\kappa}\cdot\vec{r}-\omega t\right)} = -\omega^2 \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

collect like terms: $\vec{G} + \vec{\kappa} = \vec{k} \quad \Rightarrow \quad \vec{\kappa} = \vec{k} - \vec{G}$

Central equations: $$\sum_{\vec{G}} \left(\vec{k} - \vec{G}\right)^2 b_{\vec{G}} A_{\vec{k}-\vec{G}} = \omega^2 A_{\vec{k}}$$

Plane wave method

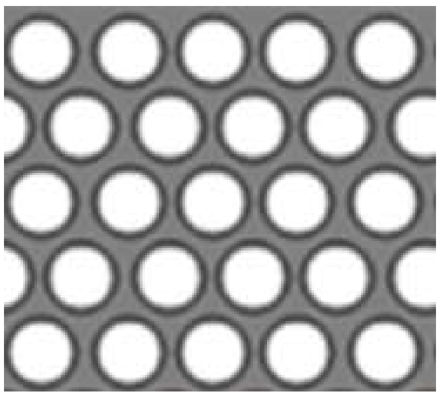
Central equations: $$\sum_{\vec{G}}\left(\vec{k}-\vec{G}\right)^2 b_{\vec{G}} A_{\vec{k}-\vec{G}} = \omega^2 A_{\vec{k}}$$

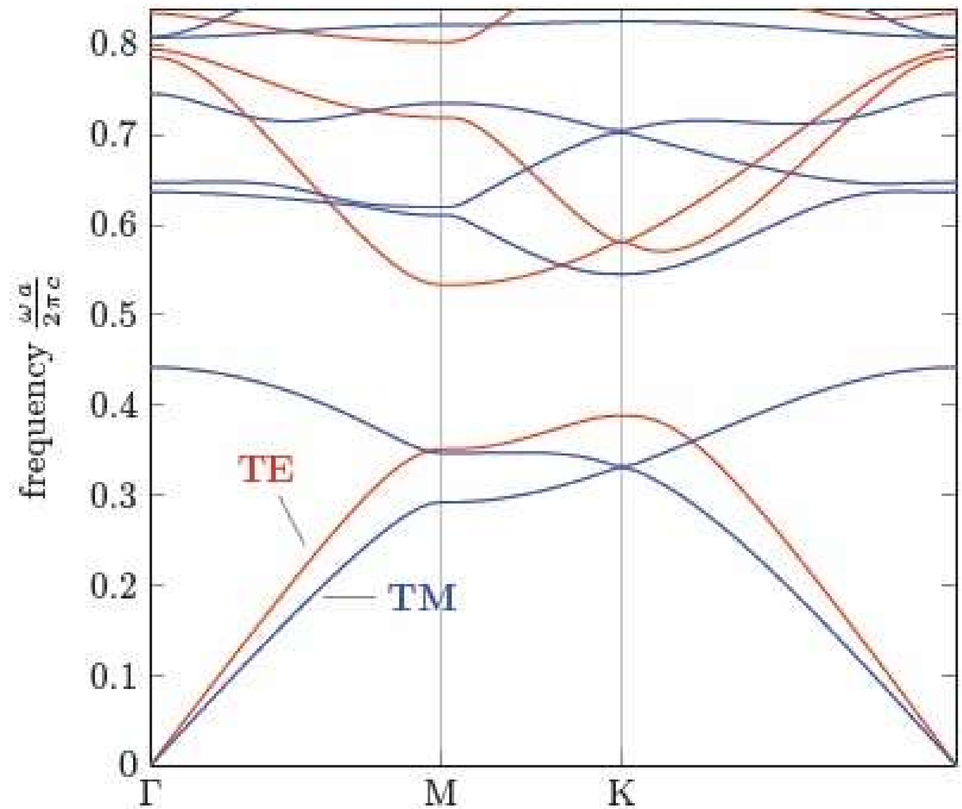
Choose a k value inside the 1st Brillouin zone. The coefficient A_k is coupled by the central equations to coefficients A_k outside the 1st Brillouin zone. Write these coupled equations in matrix form.

$$\begin{bmatrix} \left(\vec{k}+\vec{G}_2\right)^2 b_0-\omega^2 & \left(\vec{k}+\vec{G}_2-\vec{G}_1\right)^2 b_{\vec{G}_1} & k^2 b_{\vec{G}_2} & \left(\vec{k}+\vec{G}_2-\vec{G}_3\right)^2 b_{\vec{G}_3} & \left(\vec{k}+\vec{G}_2-\vec{G}_4\right)^2 b_{\vec{G}_4} \\ \left(\vec{k}+2\vec{G}_1\right)^2 b_{-\vec{G}_1} & \left(\vec{k}+\vec{G}_1\right)^2 b_0-\omega^2 & k^2 b_{\vec{G}_1} & \left(\vec{k}+\vec{G}_1-\vec{G}_2\right)^2 b_{\vec{G}_2} & \left(\vec{k}+\vec{G}_1-\vec{G}_3\right)^2 b_{\vec{G}_3} \\ \left(\vec{k}+\vec{G}_2\right)^2 b_{-\vec{G}_2} & \left(\vec{k}+\vec{G}_1\right)^2 b_{-\vec{G}_1} & k^2 b_0-\omega^2 & \left(\vec{k}-\vec{G}_1\right)^2 b_{\vec{G}_1} & \left(\vec{k}-\vec{G}_2\right)^2 b_{\vec{G}_2} \\ \left(\vec{k}-\vec{G}_1+\vec{G}_3\right)^2 b_{-\vec{G}_3} & \left(\vec{k}-\vec{G}_1+\vec{G}_2\right)^2 b_{-\vec{G}_2} & k^2 b_{-\vec{G}_1} & \left(\vec{k}-\vec{G}_1\right)^2 b_0-\omega^2 & \left(\vec{k}-2\vec{G}_1\right)^2 b_{\vec{G}_1} \\ \left(\vec{k}-\vec{G}_2+\vec{G}_4\right)^2 b_{-\vec{G}_4} & \left(\vec{k}-\vec{G}_2+\vec{G}_3\right)^2 b_{-\vec{G}_3} & k^2 b_{-\vec{G}_2} & \left(\vec{k}-\vec{G}_2+\vec{G}_1\right)^2 b_{-\vec{G}_1} & \left(\vec{k}-\vec{G}_2\right)^2 b_0-\omega^2 \end{bmatrix} \begin{bmatrix} A_{k+G_2} \\ A_{k+G_1} \\ A_k \\ A_{k-G_1} \\ A_{k-G_2} \end{bmatrix} = 0$$

There is a matrix like this for every k value in the 1st Brillouin zone.

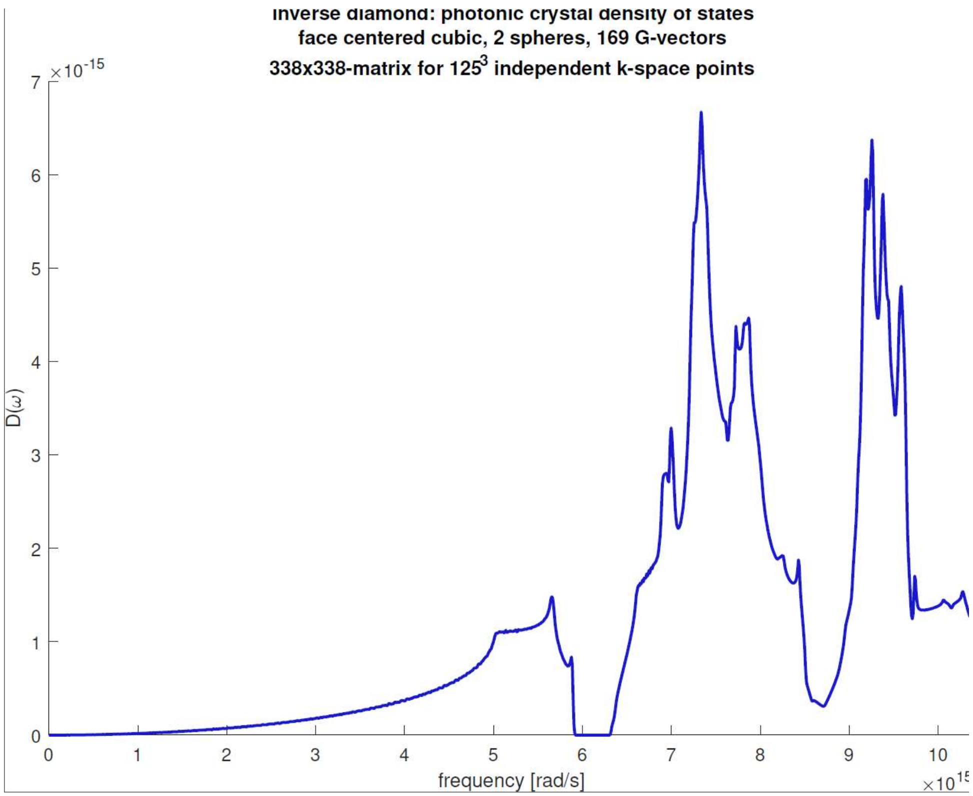
2-D array of air holes

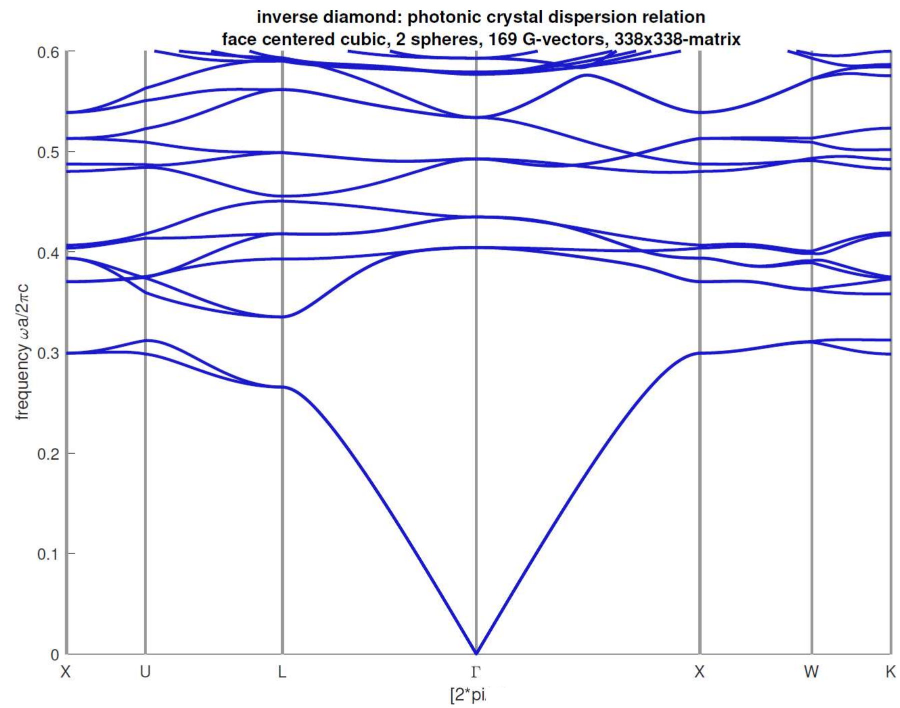


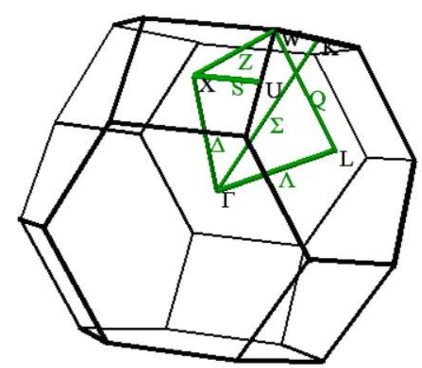


Solved by a student with the plane wave method

Inverse diamond

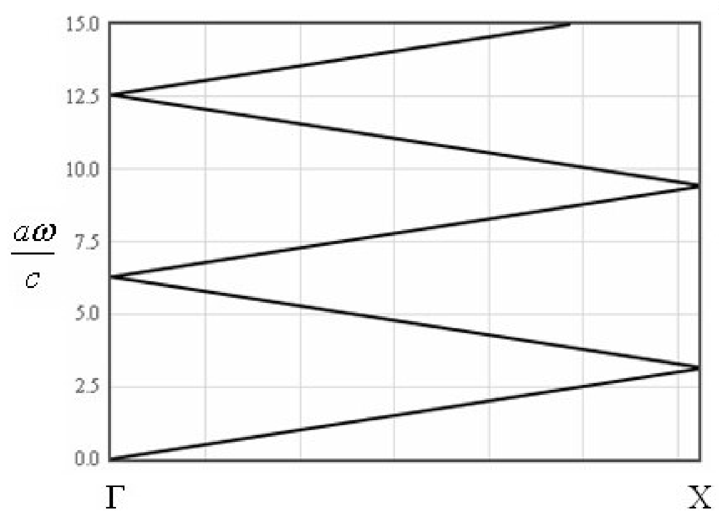


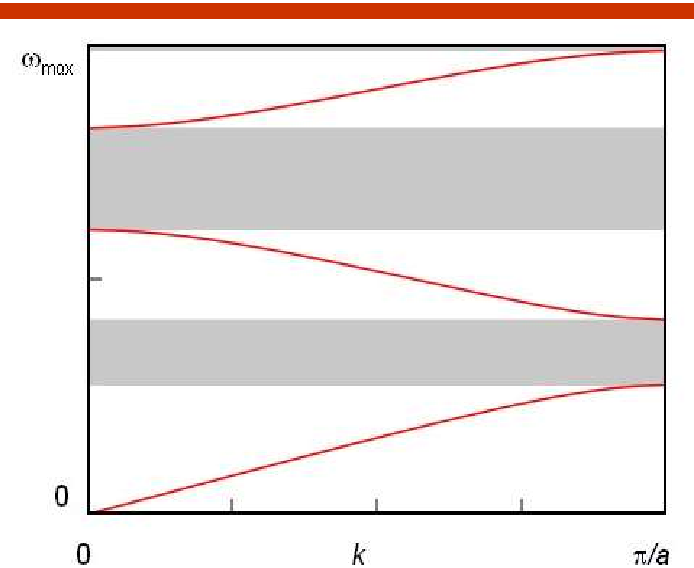


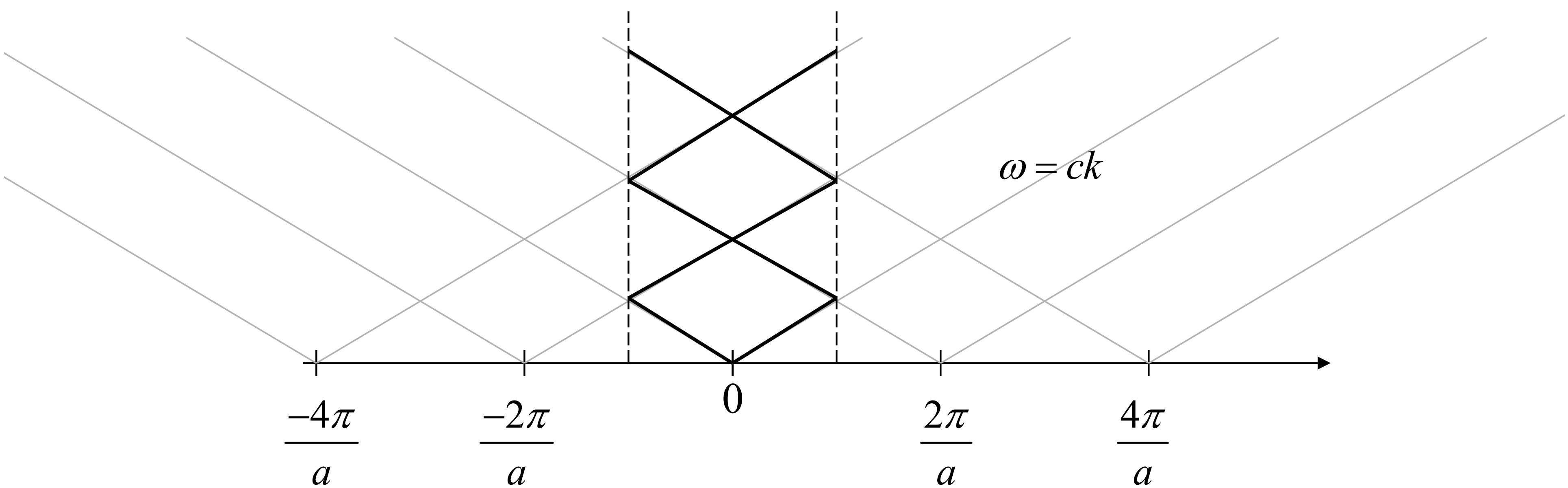


Solved by a student with the plane wave method

Empty lattice approximation

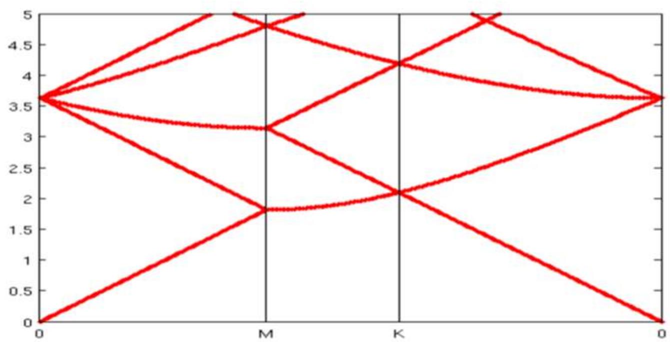


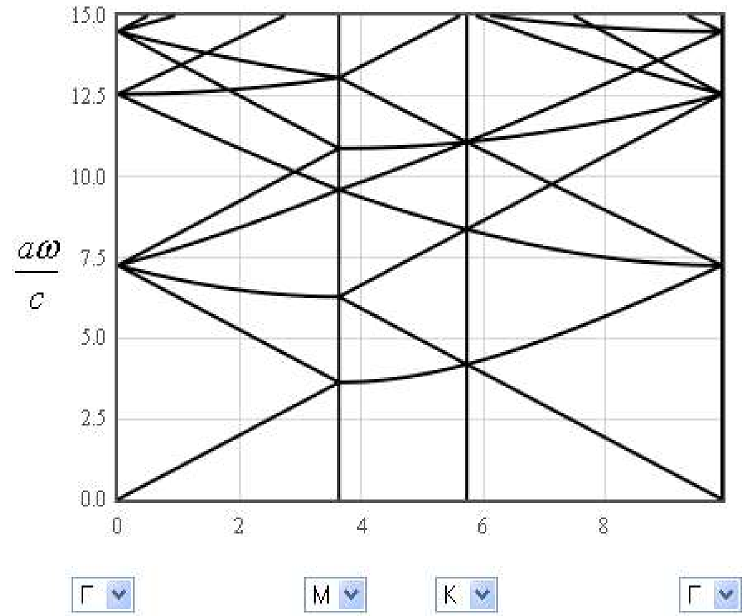


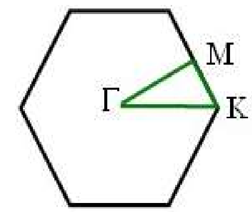


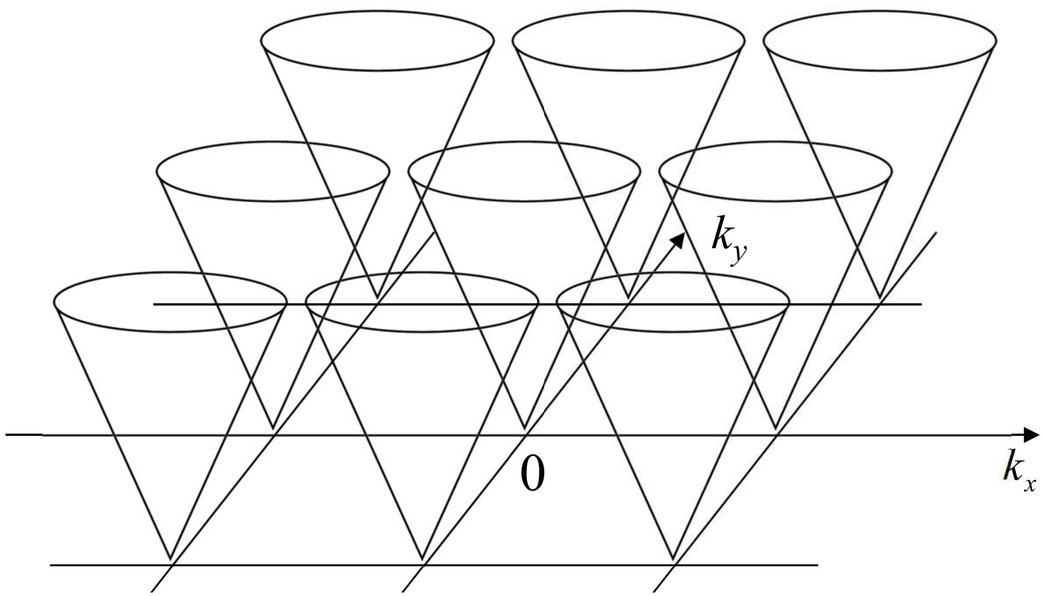
Empty lattice approximation

Plane wave method



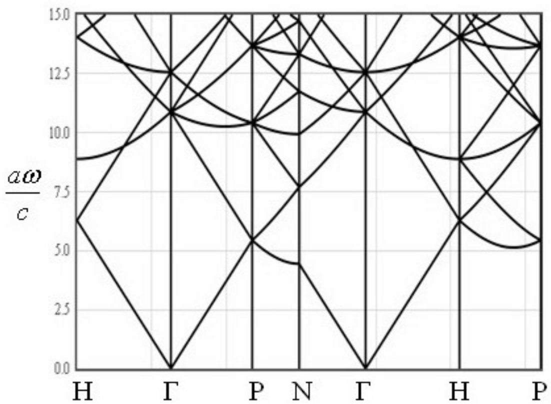




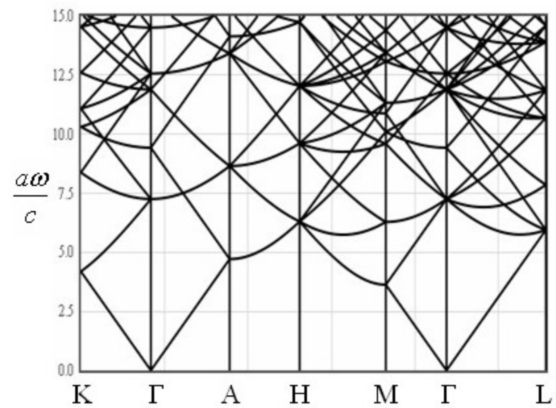


Empty lattice approximation

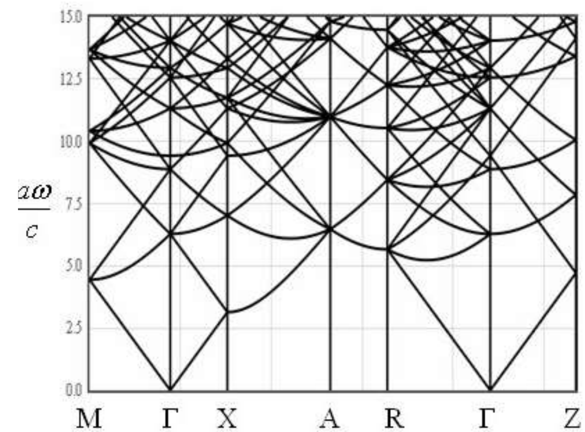
Body centered cubic

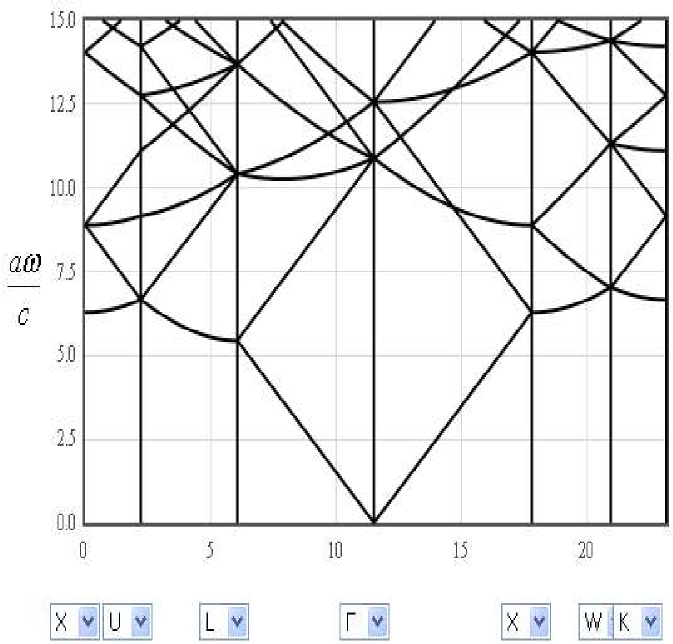


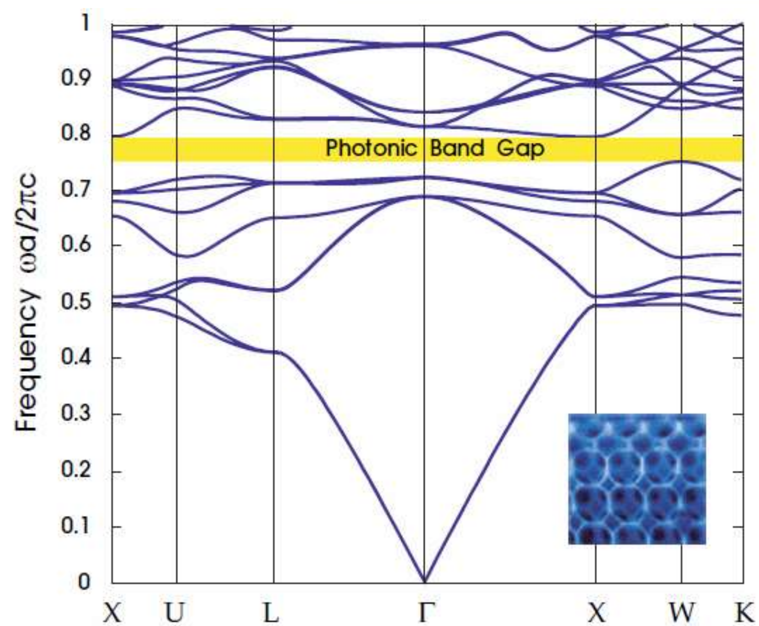
Hexagonal



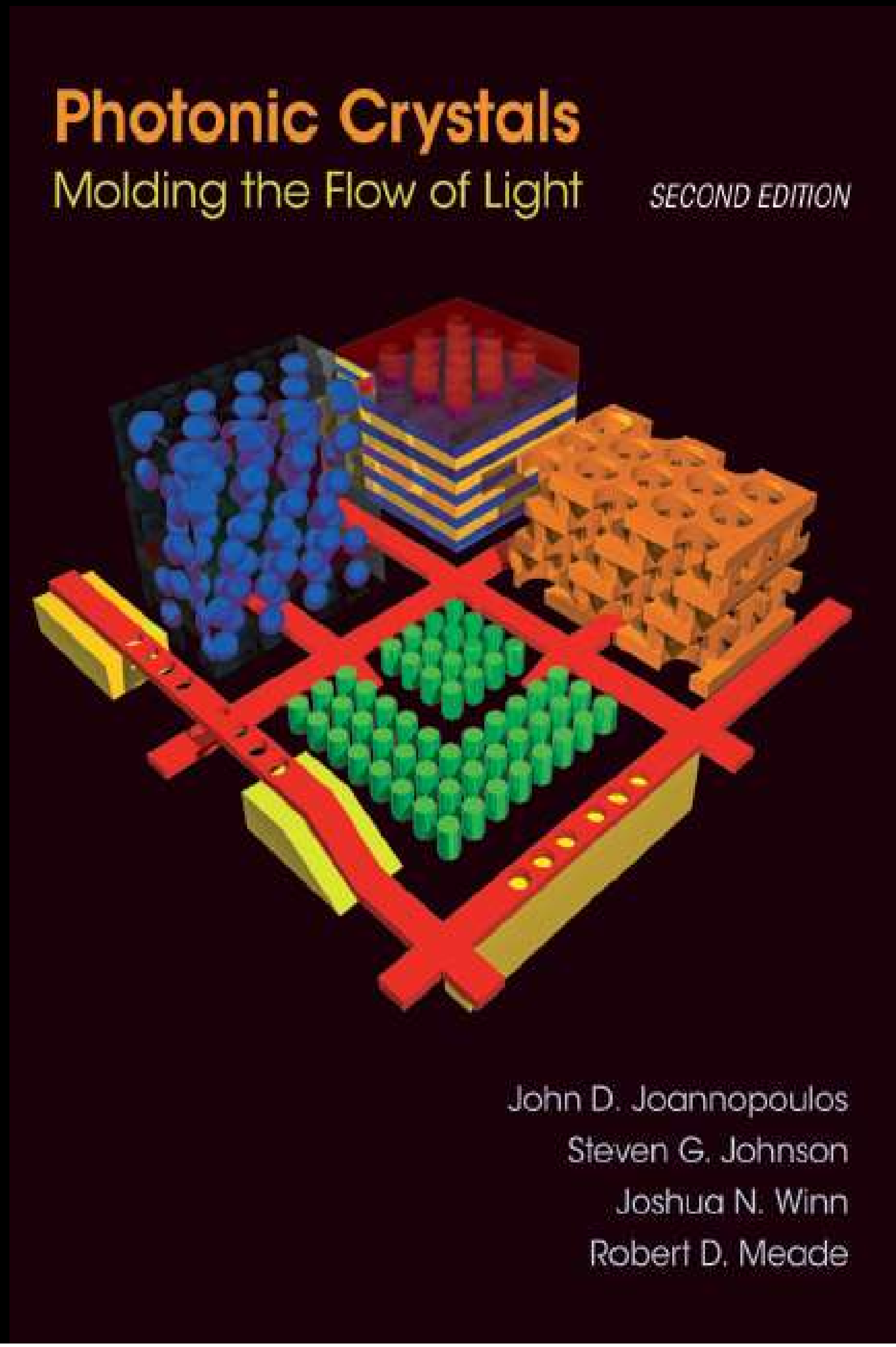
Tetragonal



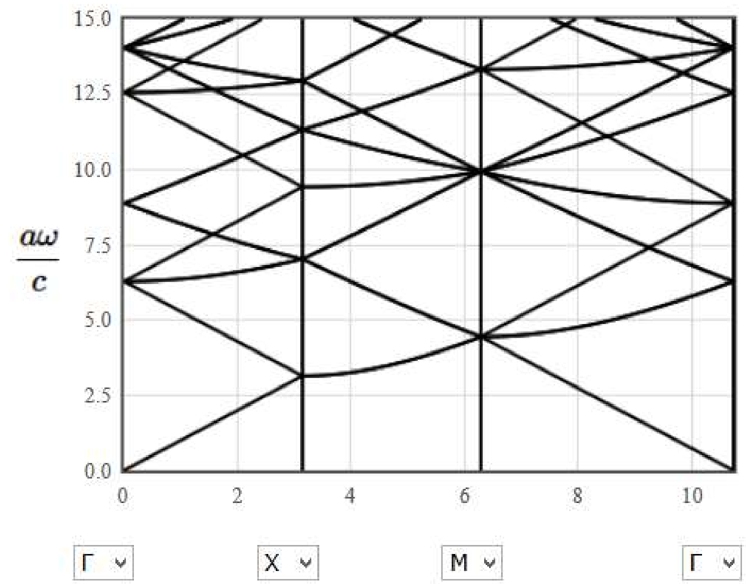


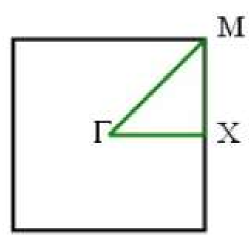


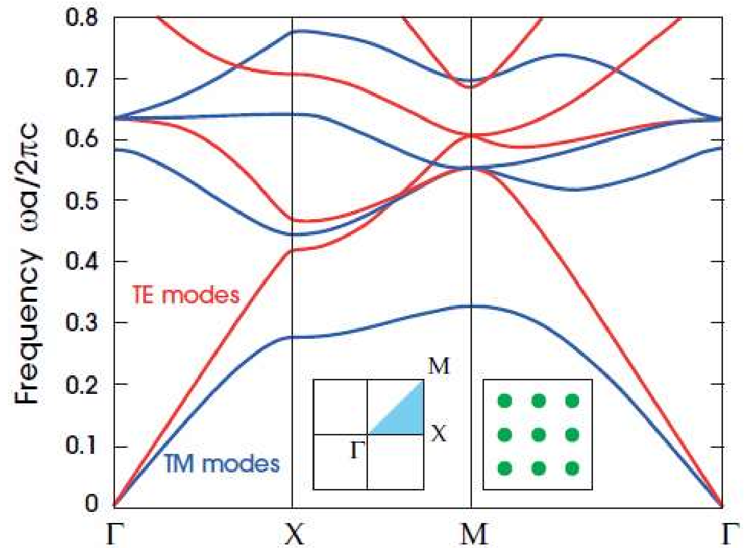
http://ab-initio.mit.edu/book/



Empty lattice approximation

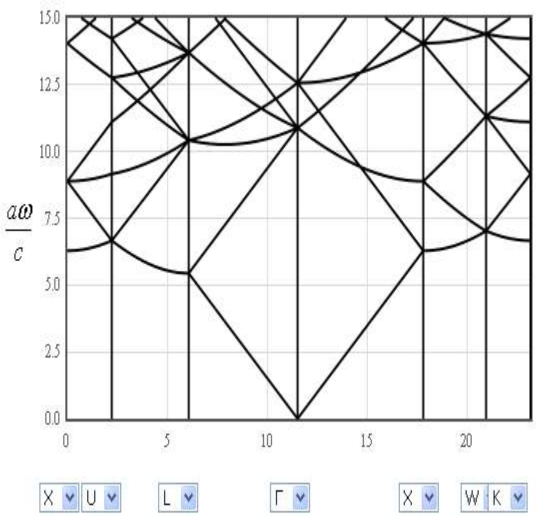






http://ab-initio.mit.edu/book/

fcc



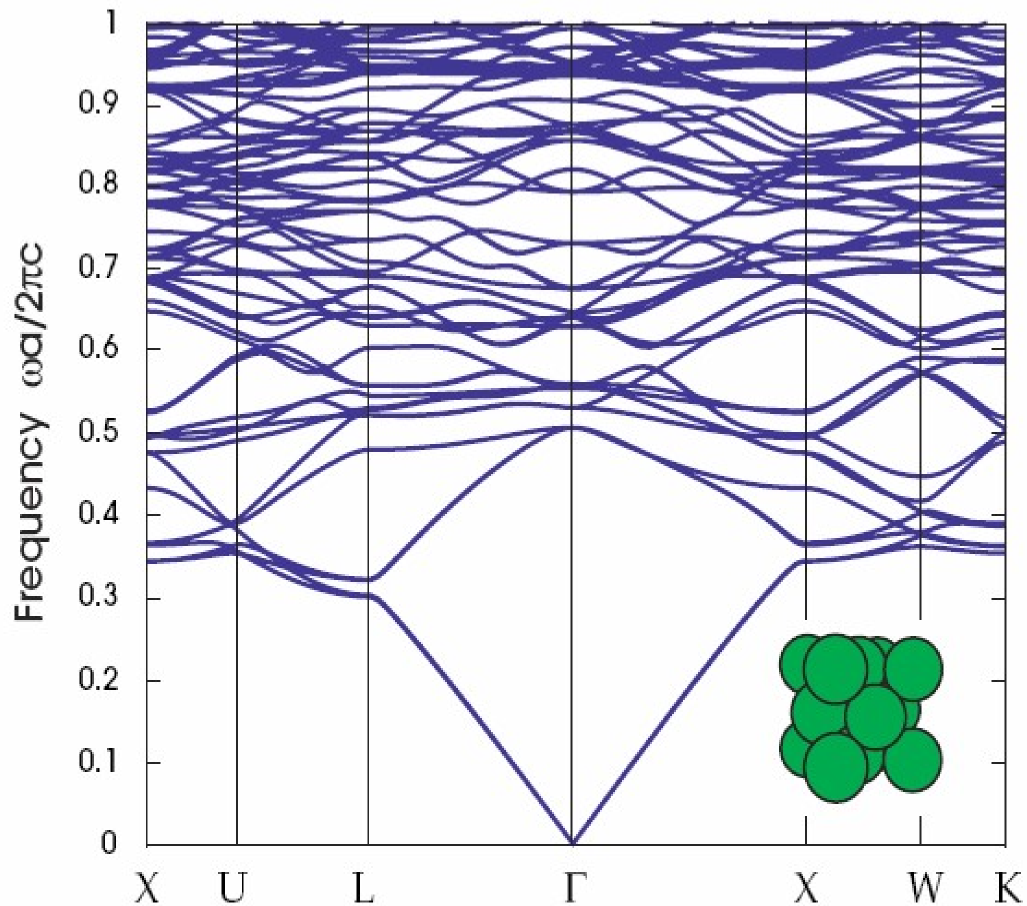
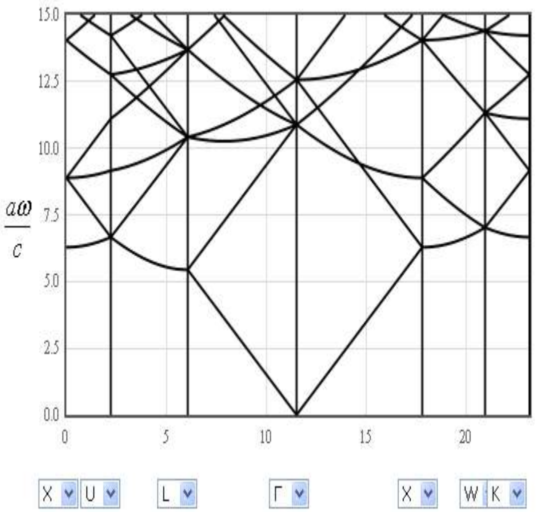


Figure 2: The photonic band structure for the lowest-frequency electromagnetic modes of a face-centered cubic (fcc) lattice of close-packed dielectric spheres ($\varepsilon = 13$) in air (inset). Note the *absence* of a complete photonic band gap. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points; see appendix B for a discussion of the Brillouin zone of an fcc lattice.

http://ab-initio.mit.edu/book/

diamond



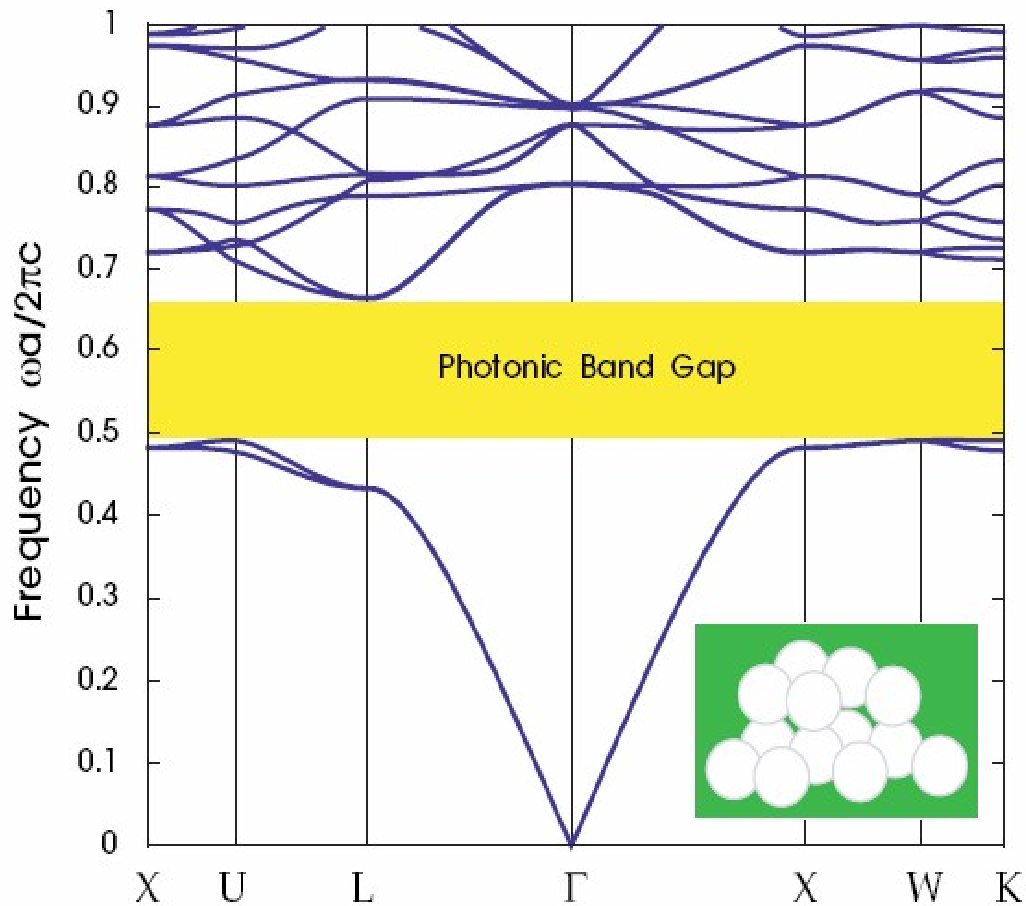
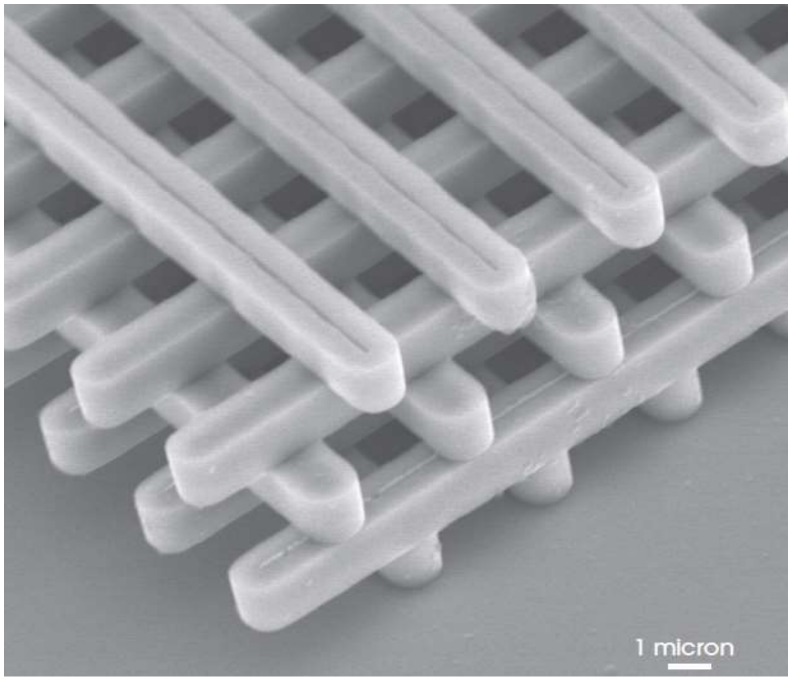


Figure 3: The photonic band structure for the lowest bands of a diamond lattice of air spheres in a high dielectric ($\varepsilon = 13$) material (inset). A complete photonic band gap is shown in yellow. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points; see appendix B for a discussion of the Brillouin zone of an fcc lattice.

http://ab-initio.mit.edu/book/

Woodpile photonic crystal



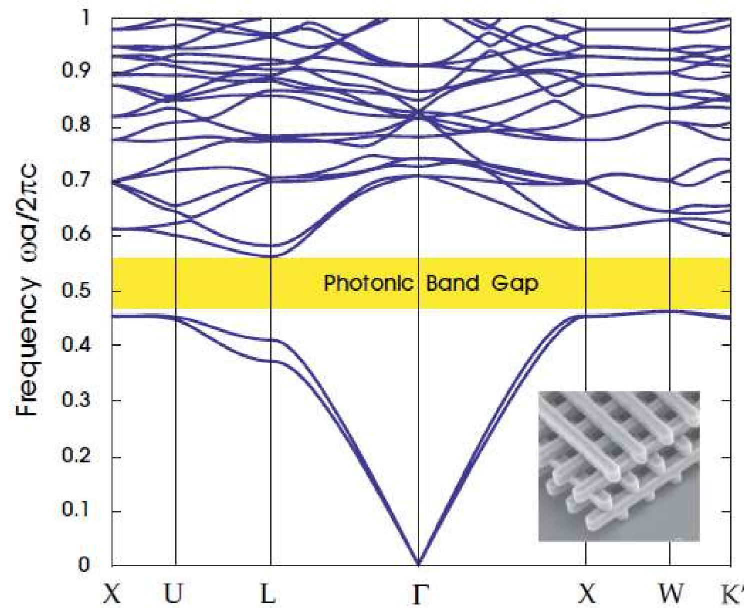
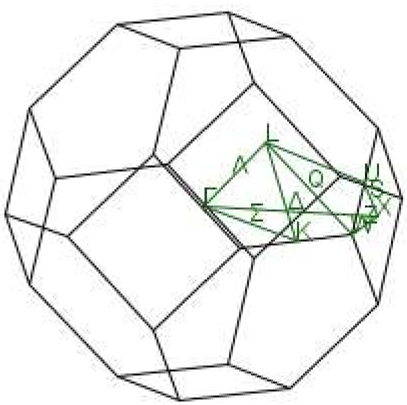
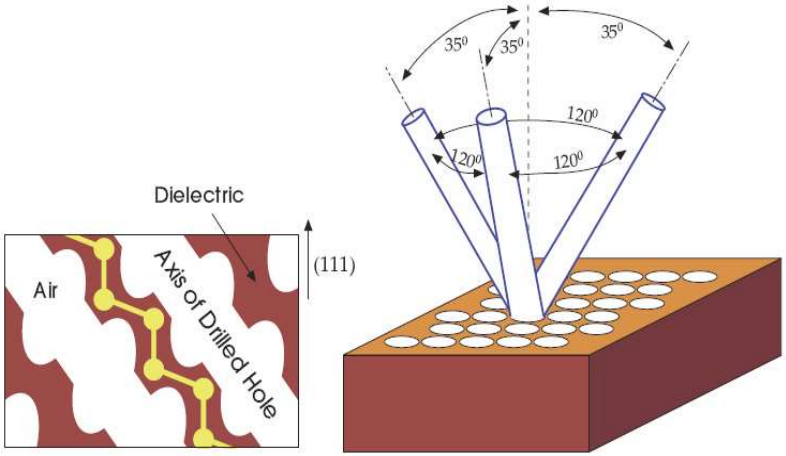


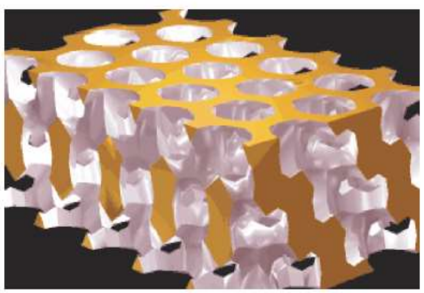
Figure 7: The photonic band structure for the lowest bands of the woodpile structure (inset, from figure 6) with $\varepsilon = 13$ logs in air. The irreducible Brillouin zone is larger than that of the fcc lattice described in appendix B, because of reduced symmetry—only a portion is shown, including the edges of the complete photonic band gap (yellow).



http://ab-initio.mit.edu/book

Yablonovite





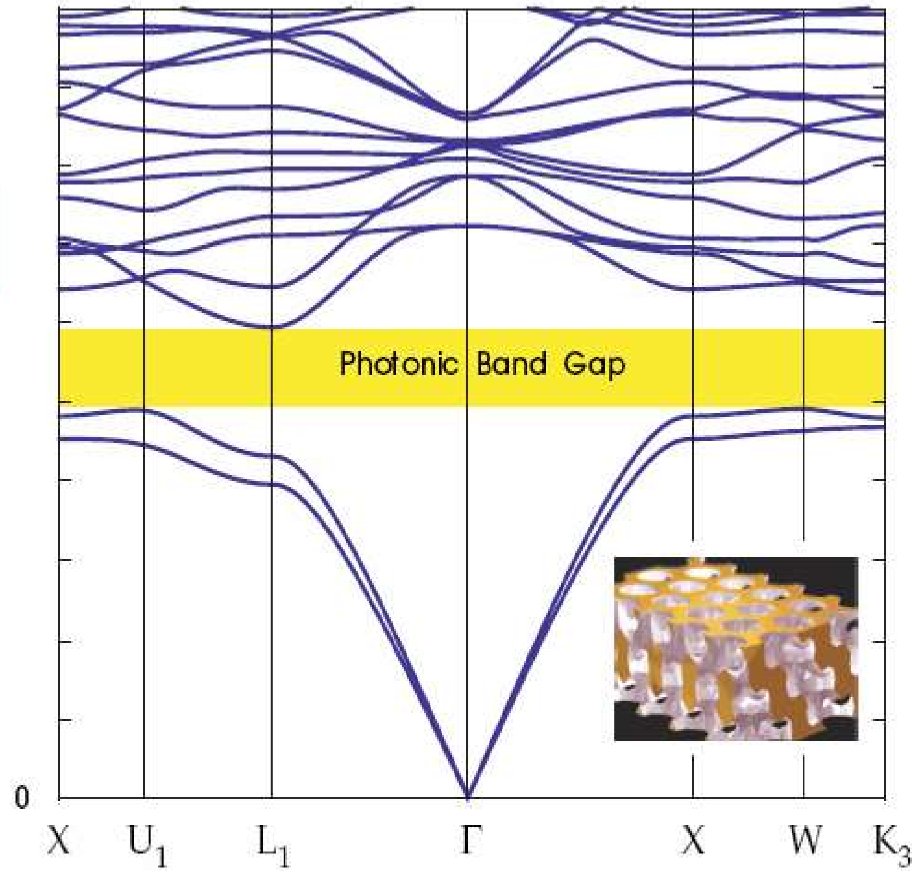
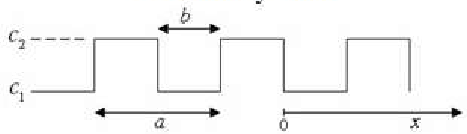


Figure 5: The photonic band structure for the lowest bands of Yablonovite (inset, from figure 4). Wave vectors are shown for a portion of the irreducible Brillouin zone that includes the edges of the complete gap (yellow). A detailed discussion of this band structure can be found in Yablonovitch et al. (1991*a*).

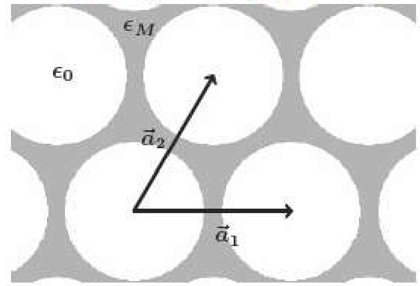
http://ab-initio.mit.edu/book/

1-D Multilayer film

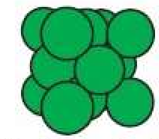


1-D Multilayer film

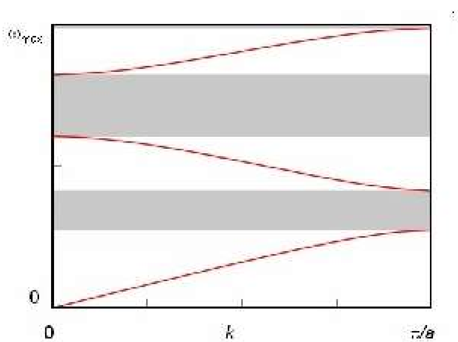
2-D triangular array of air holes



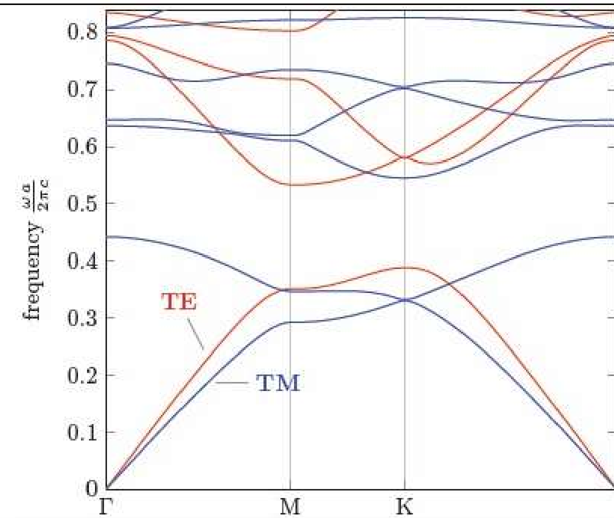
fcc

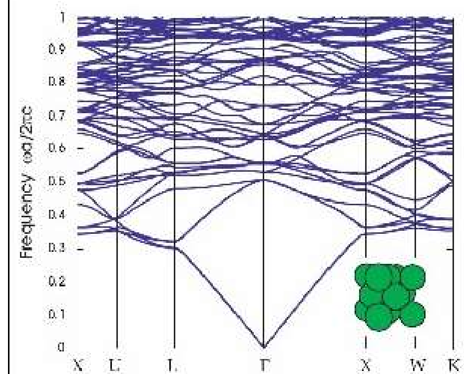


http://ab-initio.mit.edu/book

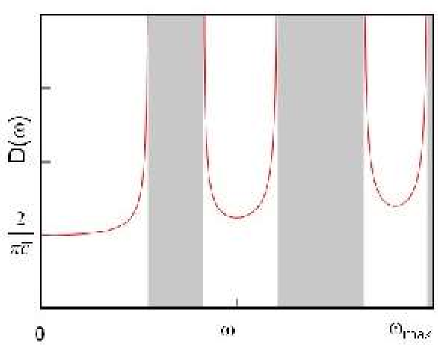


Calculate ω(k)

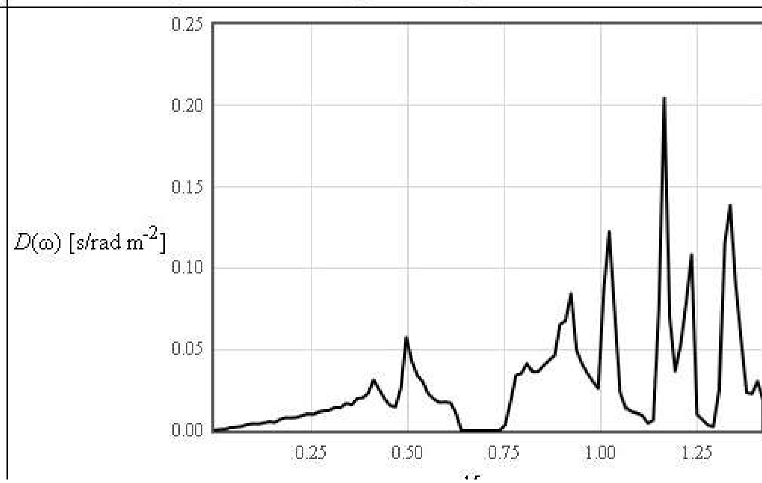




http://ab-initio.mit.edu/book



Calculate DoS



http://lampx.tugraz.at/~hadley/ss1/emfield/photonic_crystals/photonic_table.html