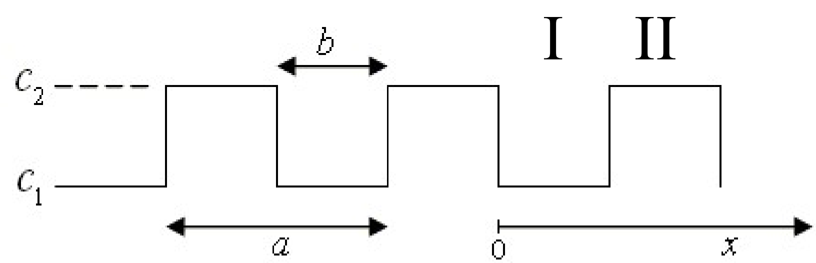
Light in a layered material



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,

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

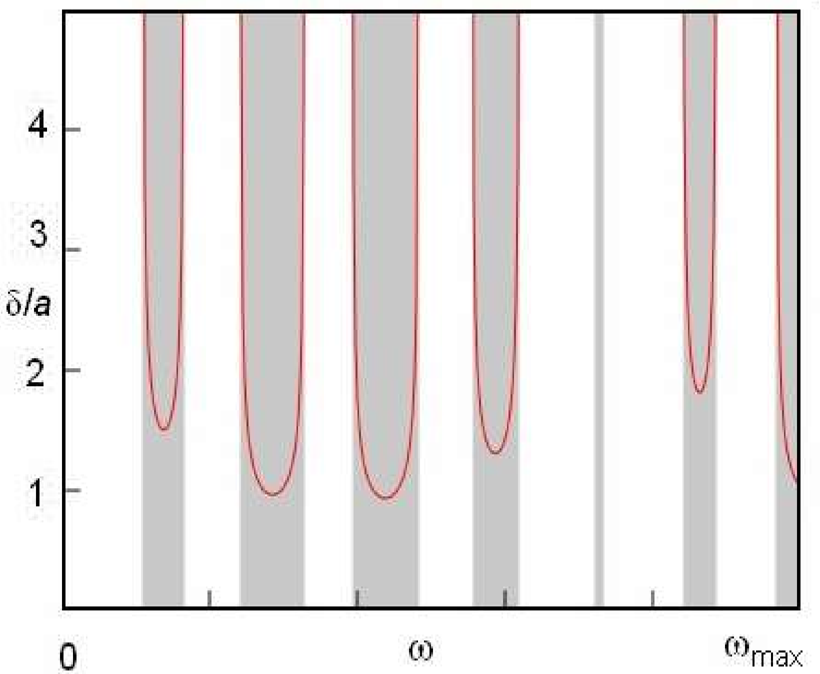
In region II,

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

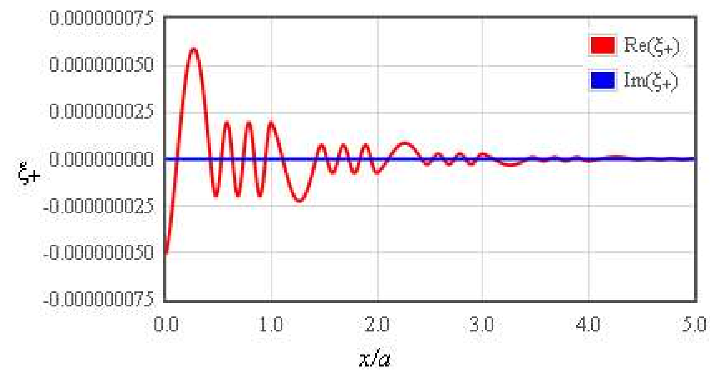
$$\xi_2(x)=\frac{c_1}{\omega}\sin\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(x-b)\right)+\frac{c_2}{\omega}\cos\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(x-b)\right)$$

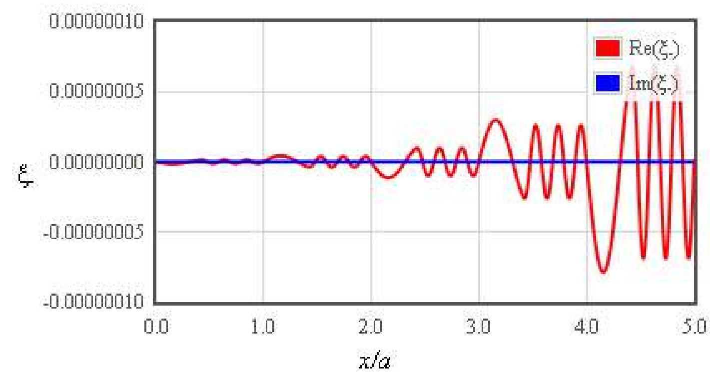
Band gap: exponentially growing solutions

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



Gray where $|\alpha| > 2$.

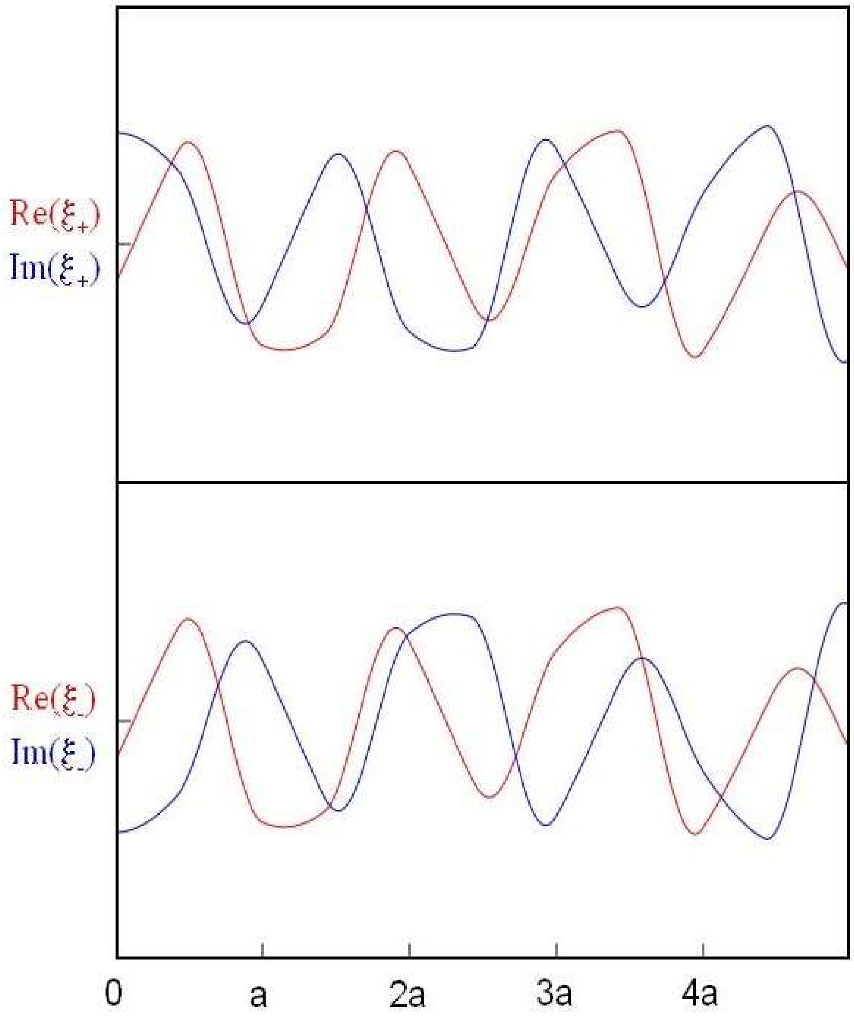




$$\delta = \frac{-a}{\ln\left(\min\left(\lambda_-, \lambda_+\right)\right)}$$

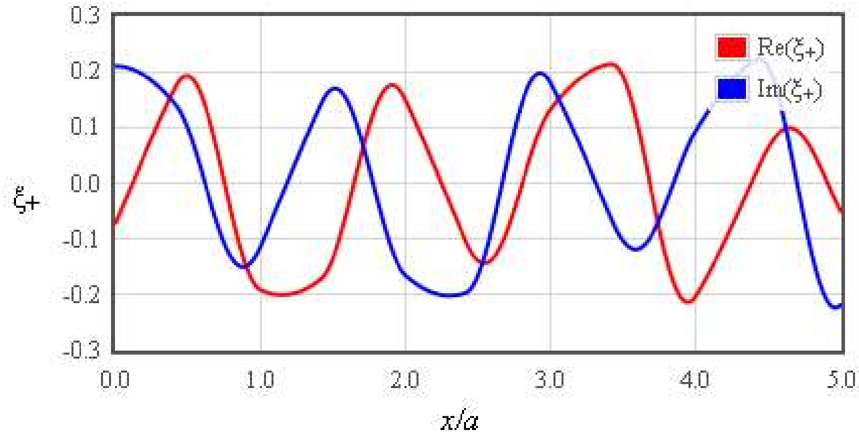
Band: Bloch waves

The solutions have the form $e^{ikx}u_k(x)$ where $u_k(x+a)=u_k(x)$

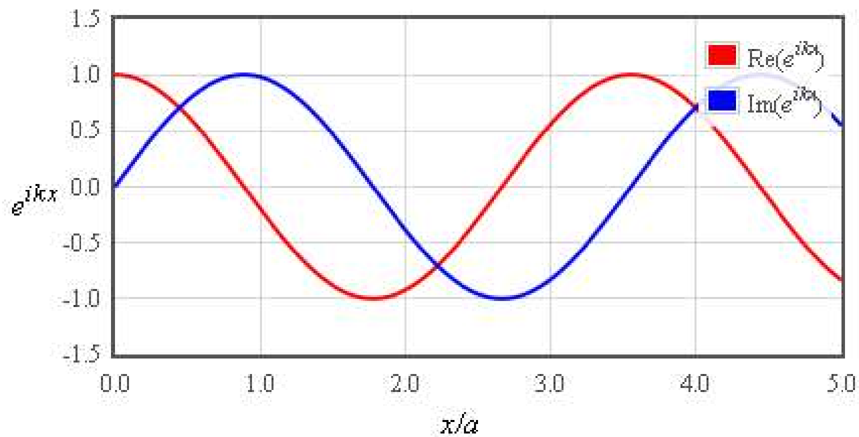


a:	600E-9	[m]
b:	250E-9	[m]
c_1:	2.998E8	[m/s]
c_2:	1E8	[m/s]
ω:	1E15	[rad/s]

Bloch waves

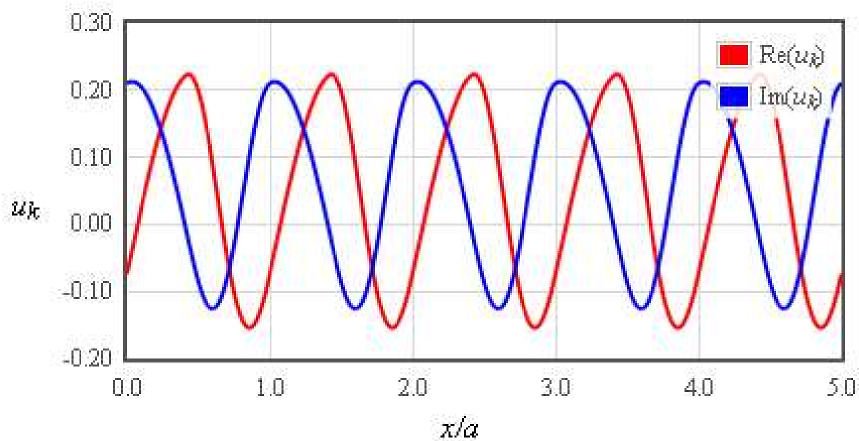


$$\xi = e^{ikx} u_k(x)$$



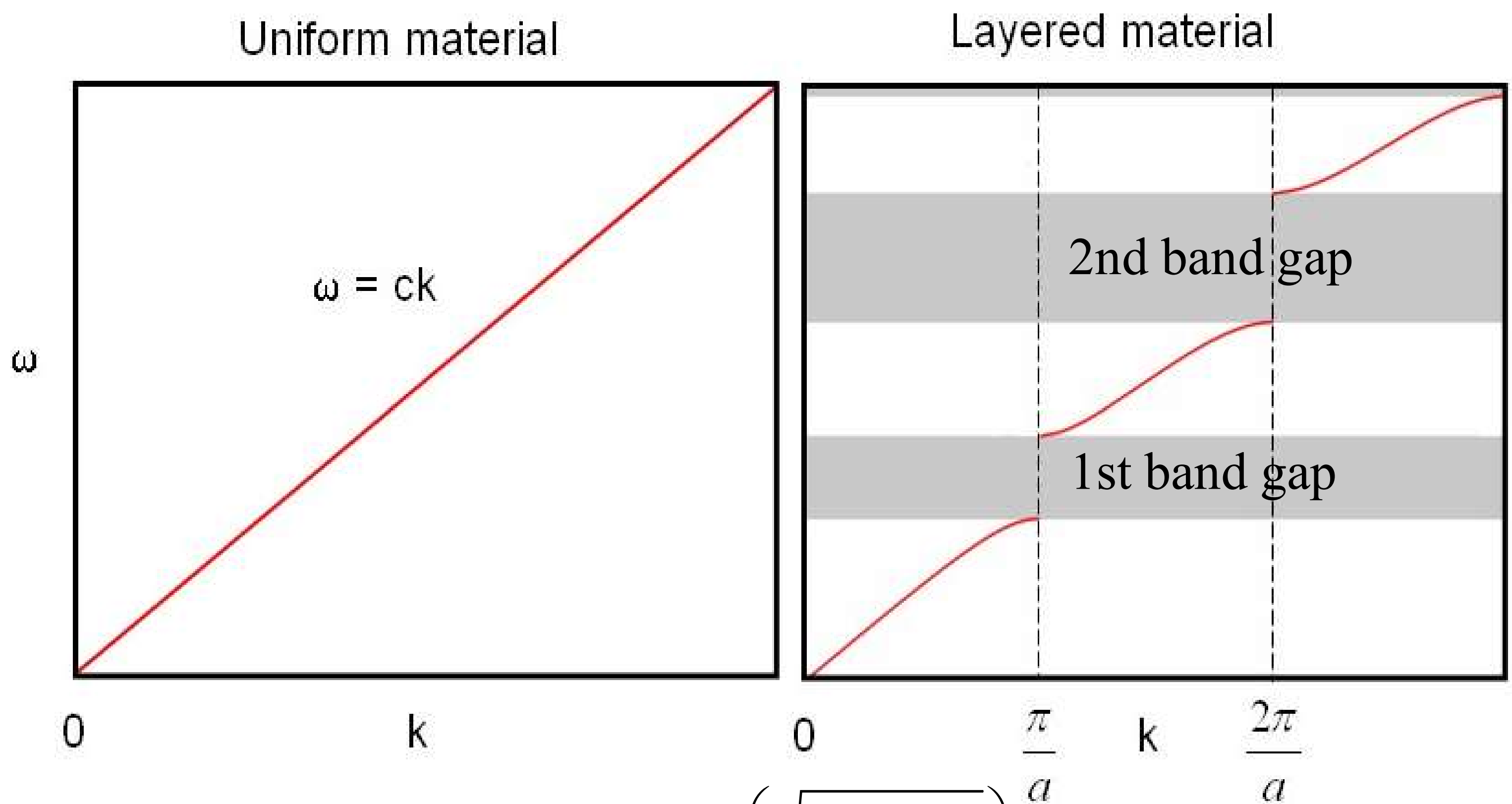
For periodic boundary conditions $L = Na$, the allowed values of k are exactly those allowed for waves in vacuum.

k labels the eigenfunctions of the translation operator.



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

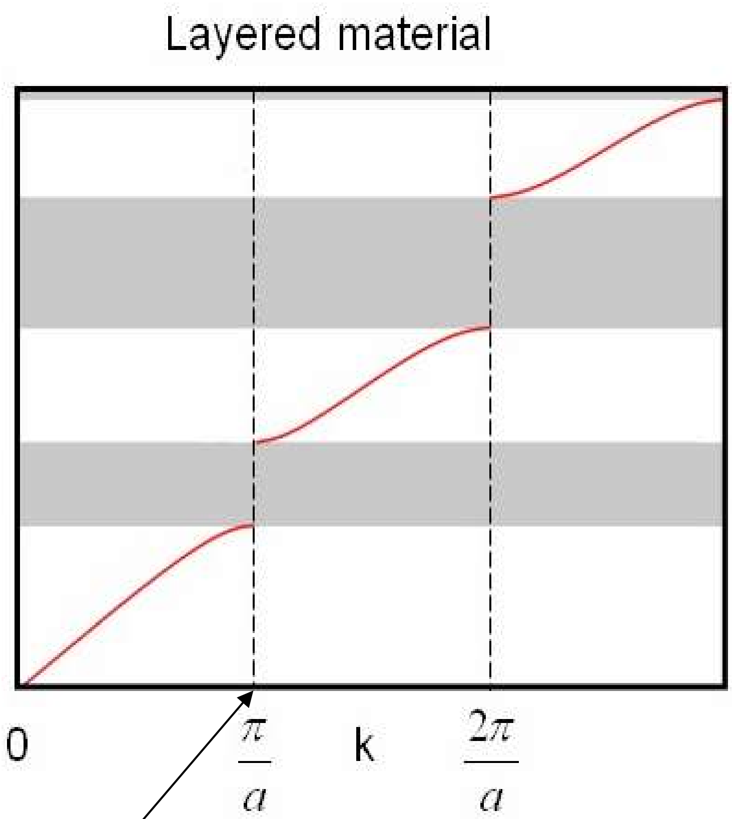
Dispersion relation

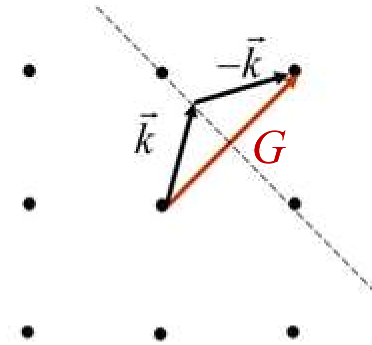


$$k = \frac{1}{a}\tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2} - 1}\right)$$

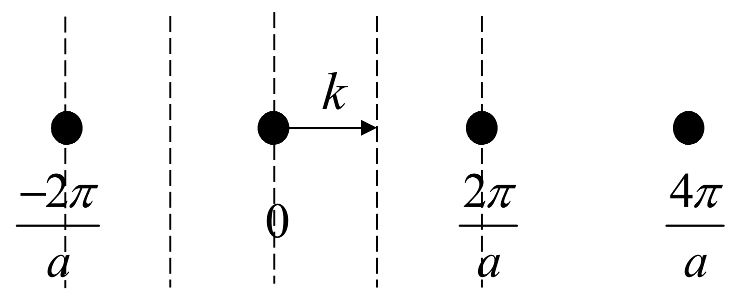
$$\alpha(\omega) = 2\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(a-b)\right) - \frac{c_1^2 + c_2^2}{c_1 c_2}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(a-b)\right)$$

Diffraction condition



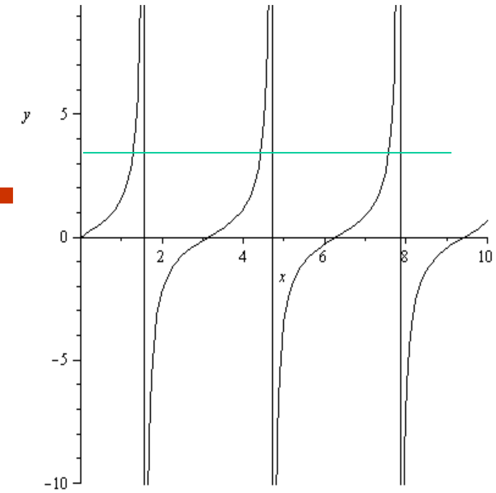


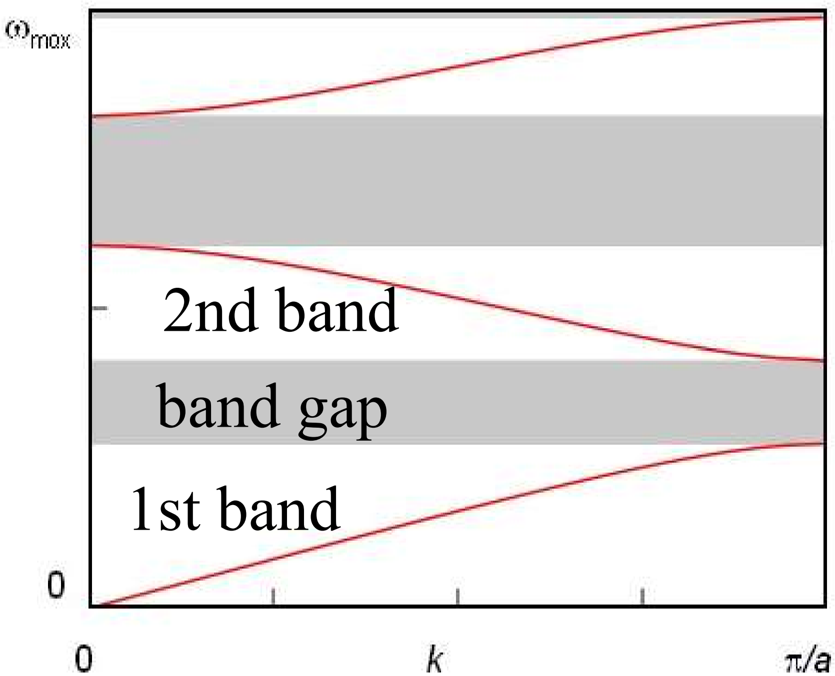
1st Brilluoin zone boundary



Dispersion relation

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





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

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

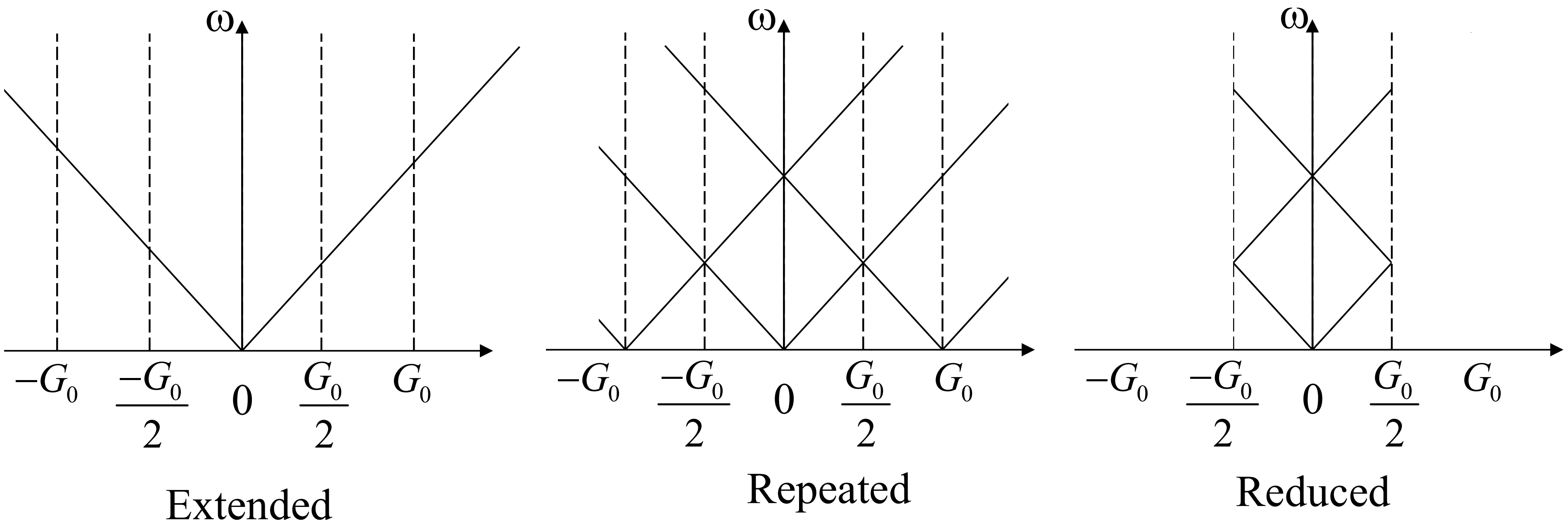
$$k = k' + G'$$

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

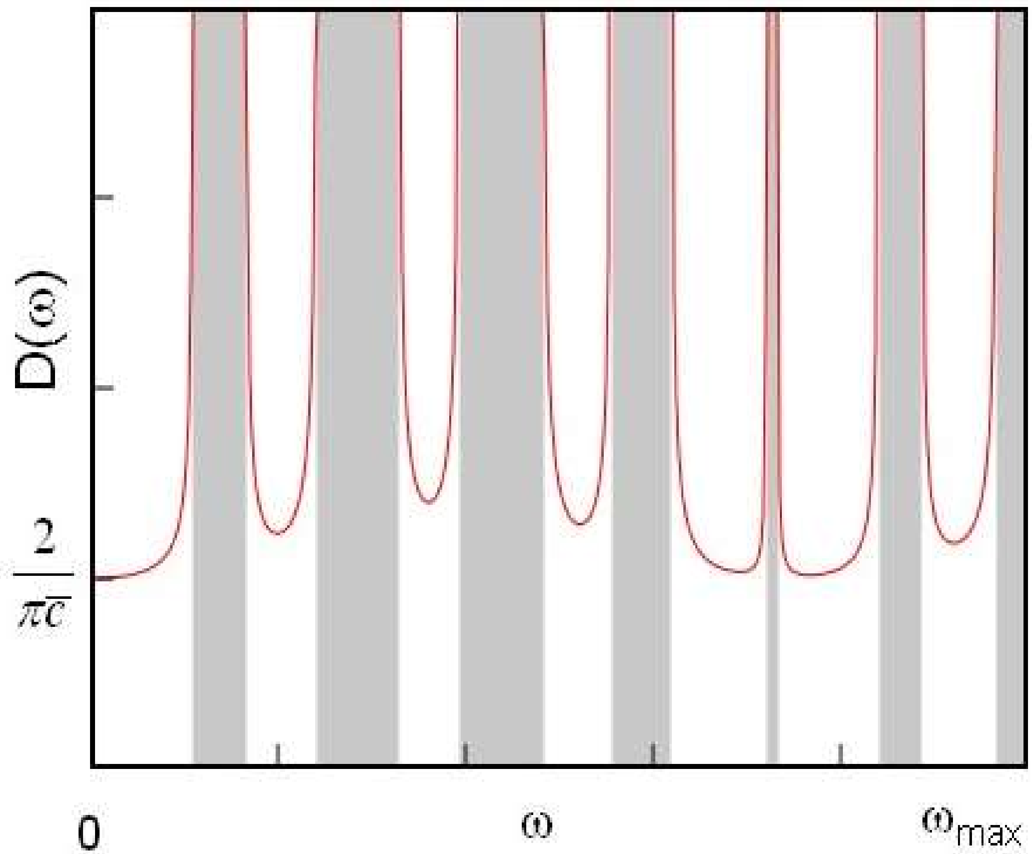
$$e^{ikx}u_k(x) = e^{ik'x}\sum_G a_G e^{i(G+G')x}$$

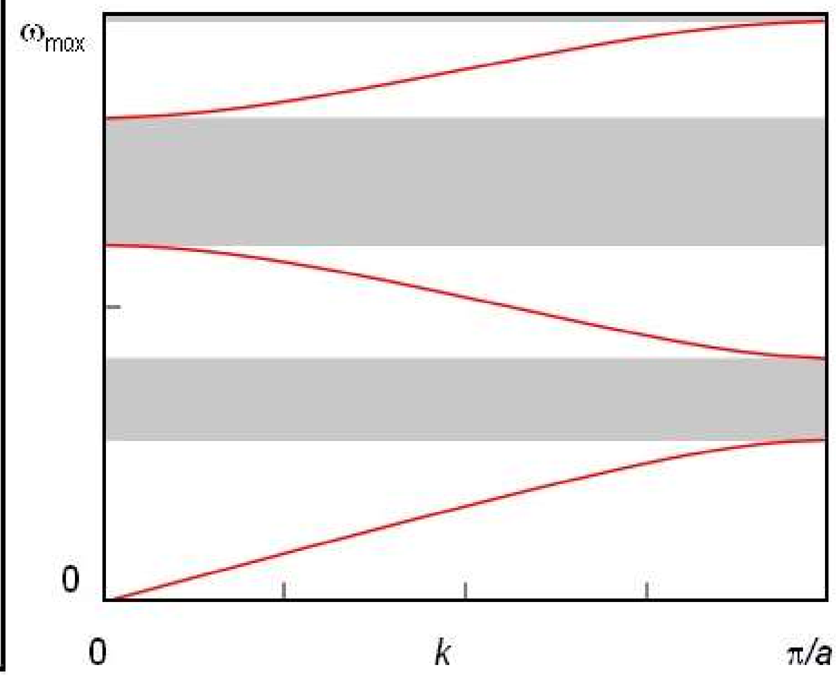
There is only one k' in the first Brillouin zone and the convention is to use that one.

Zone schemes



Density of states

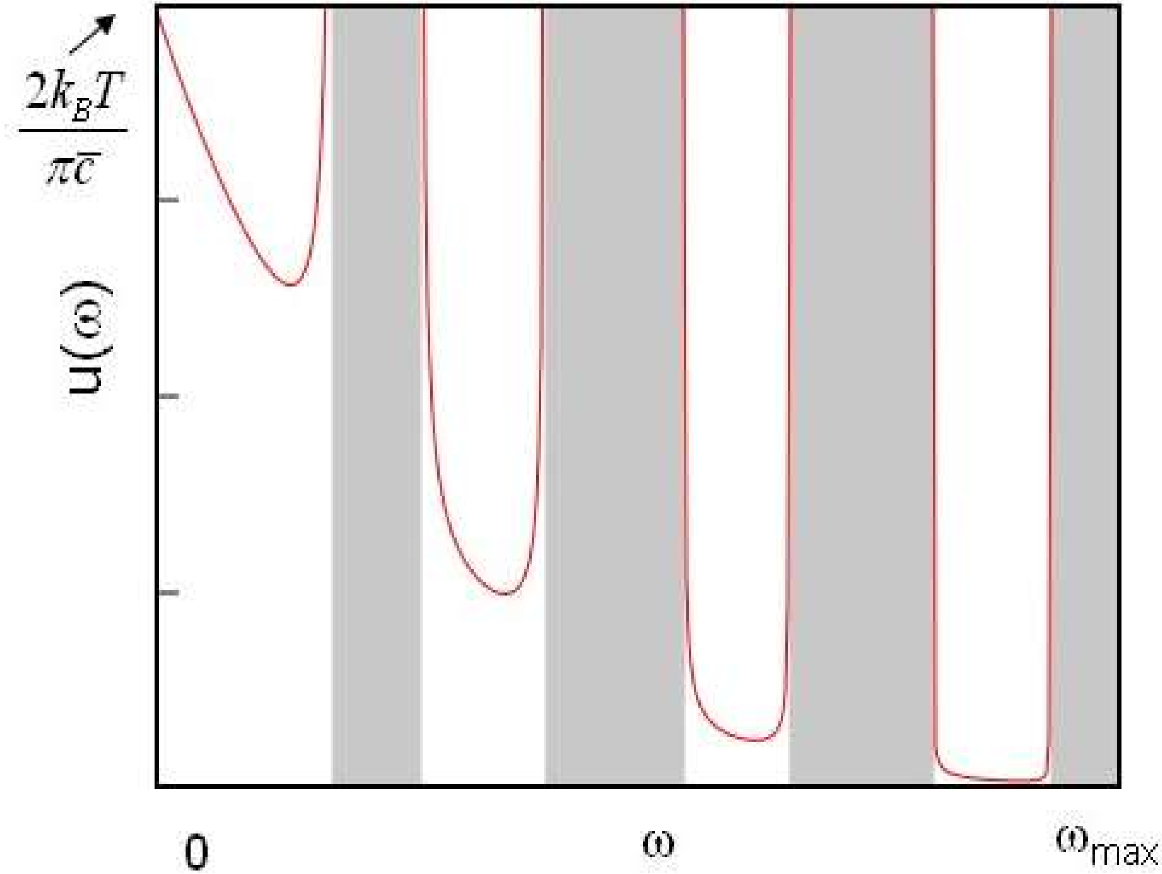




$$D(\omega) = D(k)\frac{dk}{d\omega}$$

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

Energy spectral density



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

Analog to the Planck radiation curve.

Thermodynamic quantities

Energy spectral density:

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

DoS → u(ω)

Internal energy density:

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

DoS → u(T)

Helmholz free energy density:

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

DoS → f(T)

Entropy density:

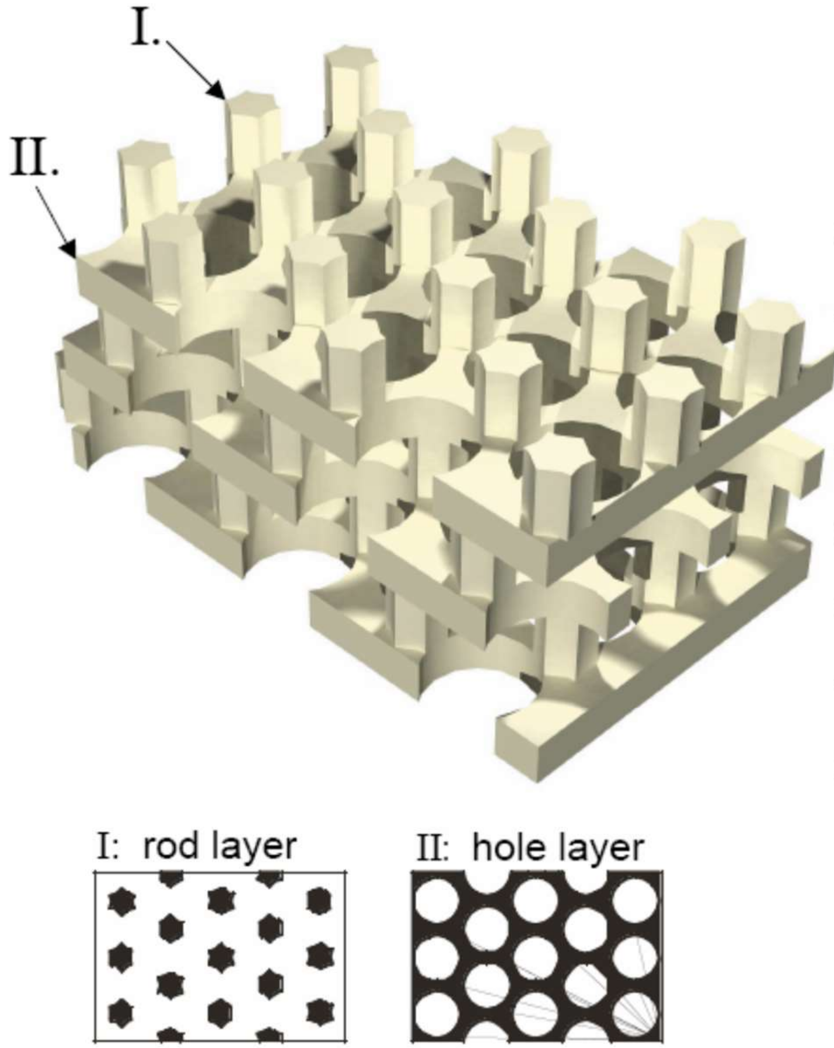
$$s=-\frac{\partial f}{\partial T}=k_B\int_0^\infty D(\omega)\left(\ln\left(1-e^{-\hbar\omega/k_BT}\right)+\frac{\hbar\omega e^{-\hbar\omega/k_BT}}{k_BT\left(e^{-\hbar\omega/k_BT}-1\right)}\right)d\omega$$

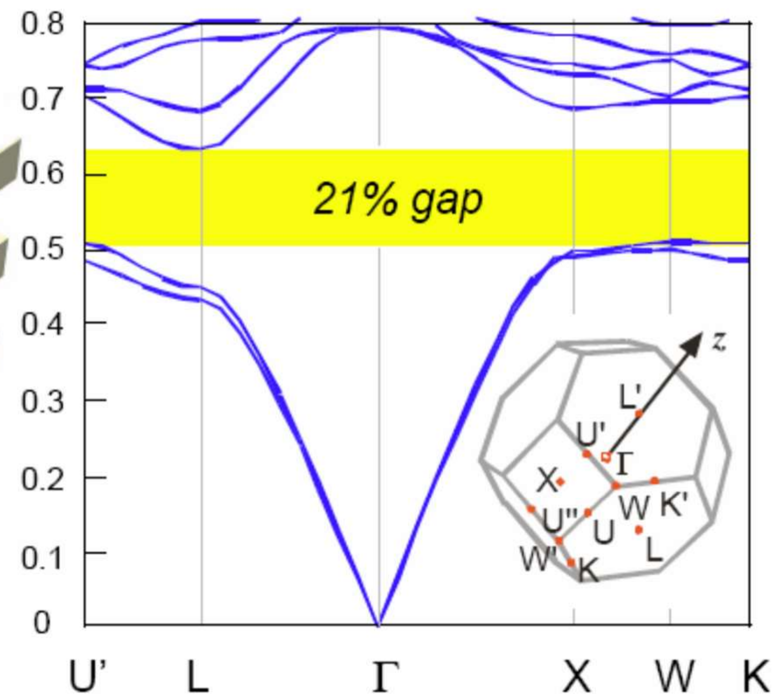
Specific heat:

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

DoS → cv(T)

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



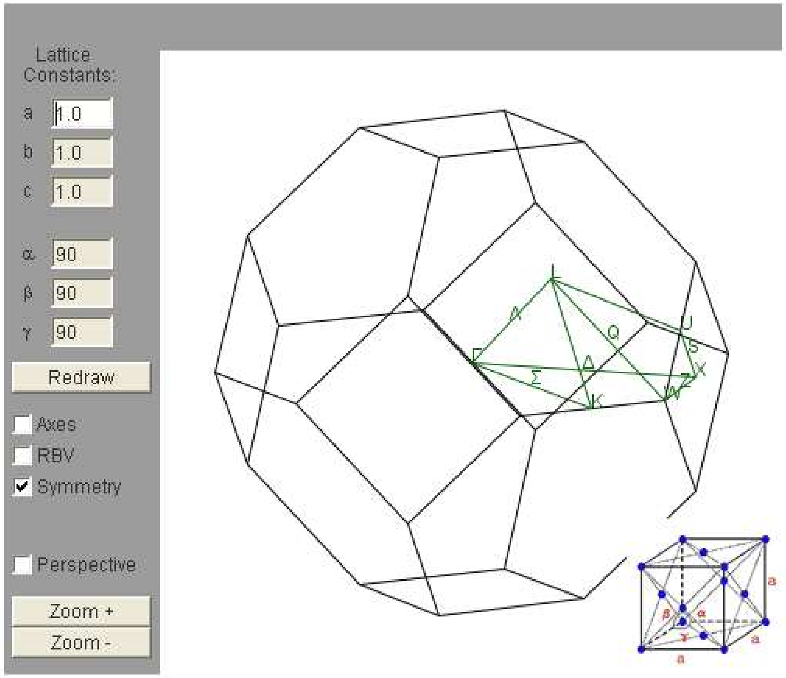


gap for n > ~4:1

[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)	[kx,ky,kz]	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

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

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

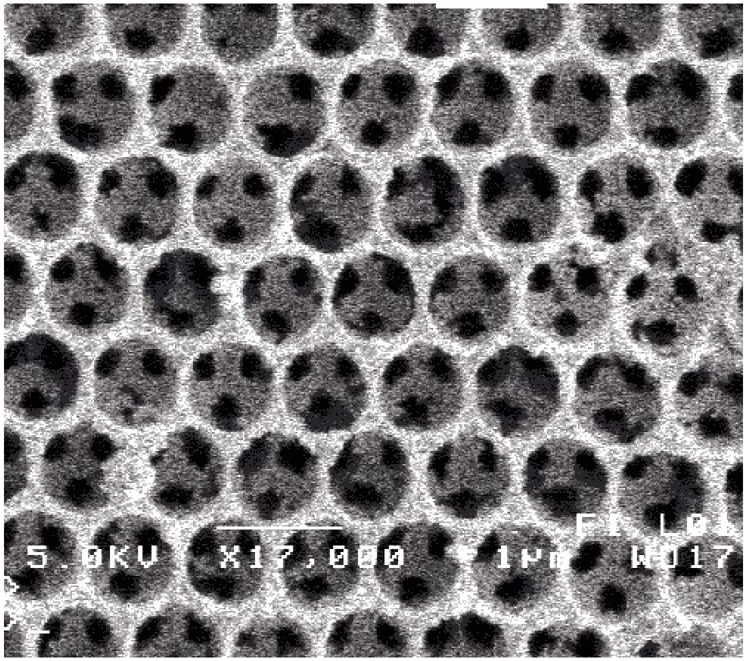
Symmetry lines	Point group
Δ: (0,v,v) 0 < v < 1/2	4mm
Λ: (w,w,w) 0 < w < 1/2	3m
Σ: (u,2u,u) 0 < u < 3/8	mm2
S: (2u,1/2+2u,1/2+u) 0 < u < 1/8	mm2
Z: (u,1/2+u,1/2) 0 < u < 1/4	mm2
Q: (1/2-u,1/2+u,1/2) 0 < u < 1/4	2

The real space and reciprocal space primitive translation vectors are:

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

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

Inverse opal photonic crystal



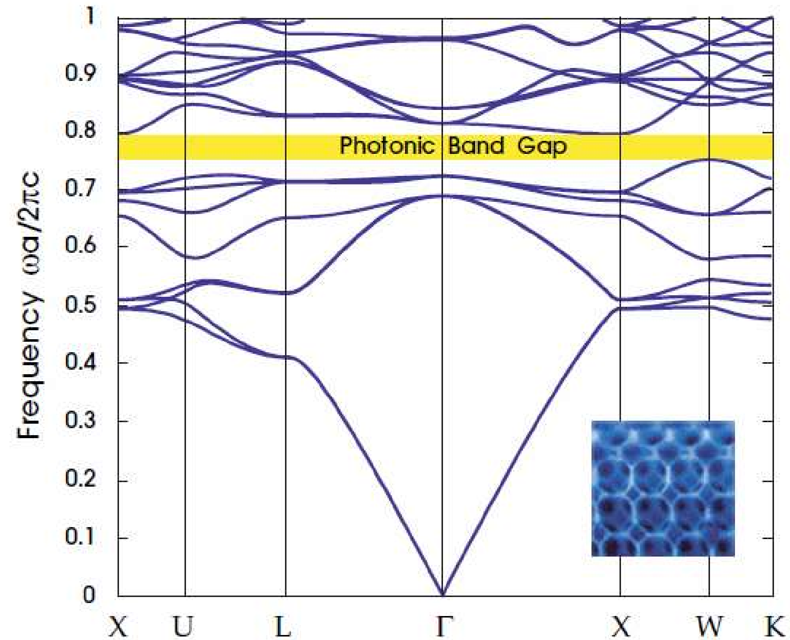
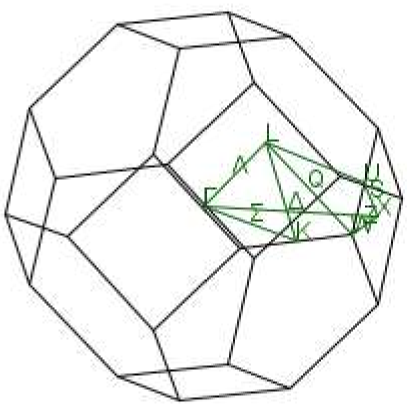


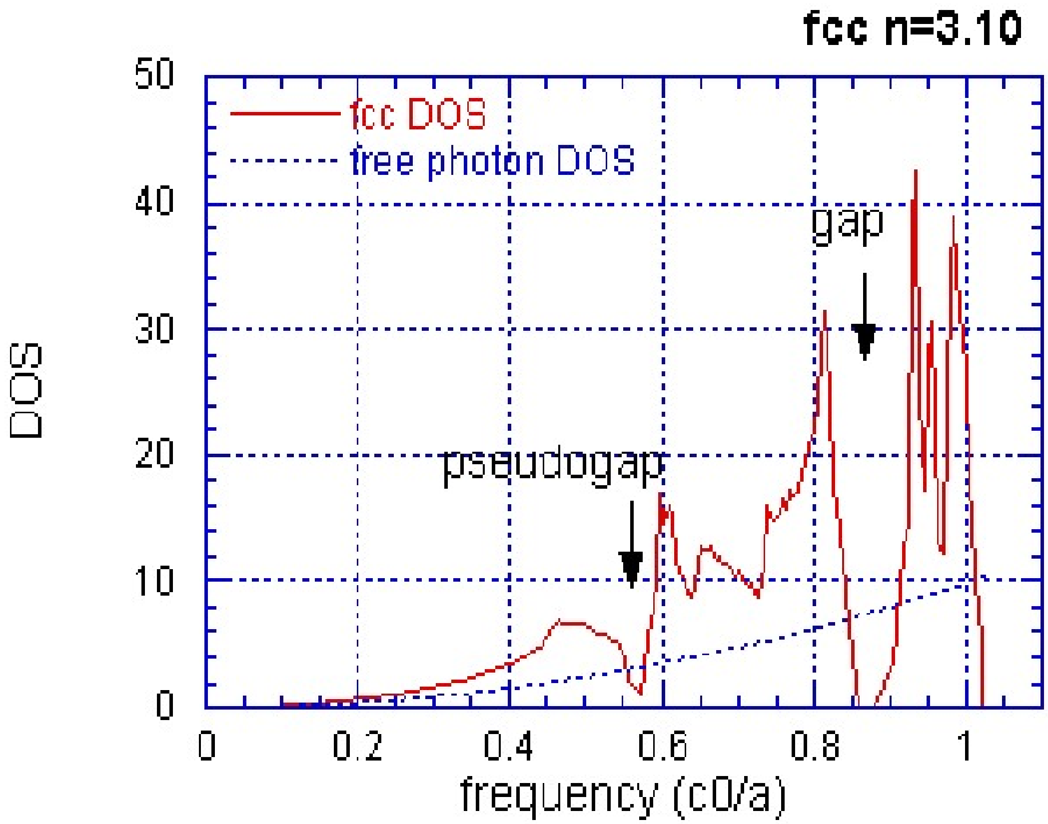
Figure 8: The photonic band structure for the lowest bands of an "inverse opal" structure: a face-centered cubic (fcc) lattice of close-packed air spheres in dielectric ($\varepsilon = 13$). (Inset shows fabricated structure from figure 9.) There is a complete photonic band gap (yellow) between the eighth 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.

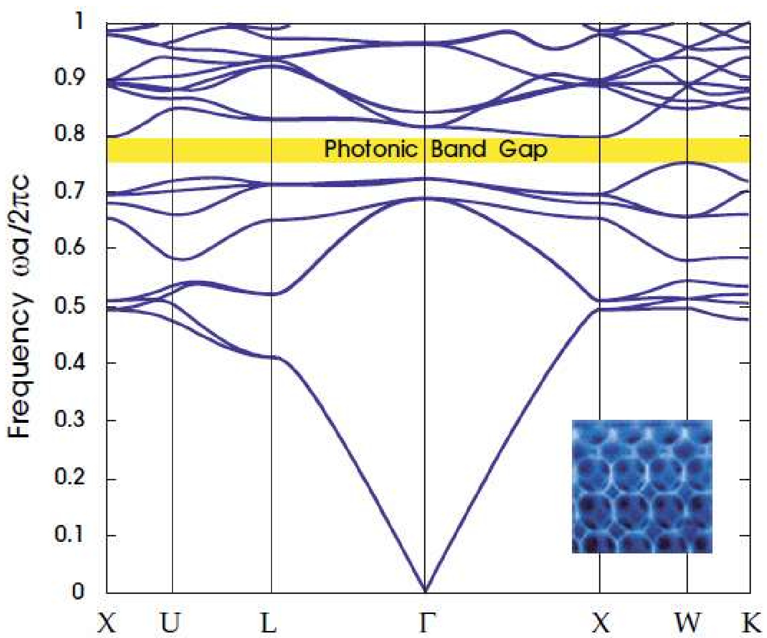


http://ab-initio.mit.edu/book

Photon density of states

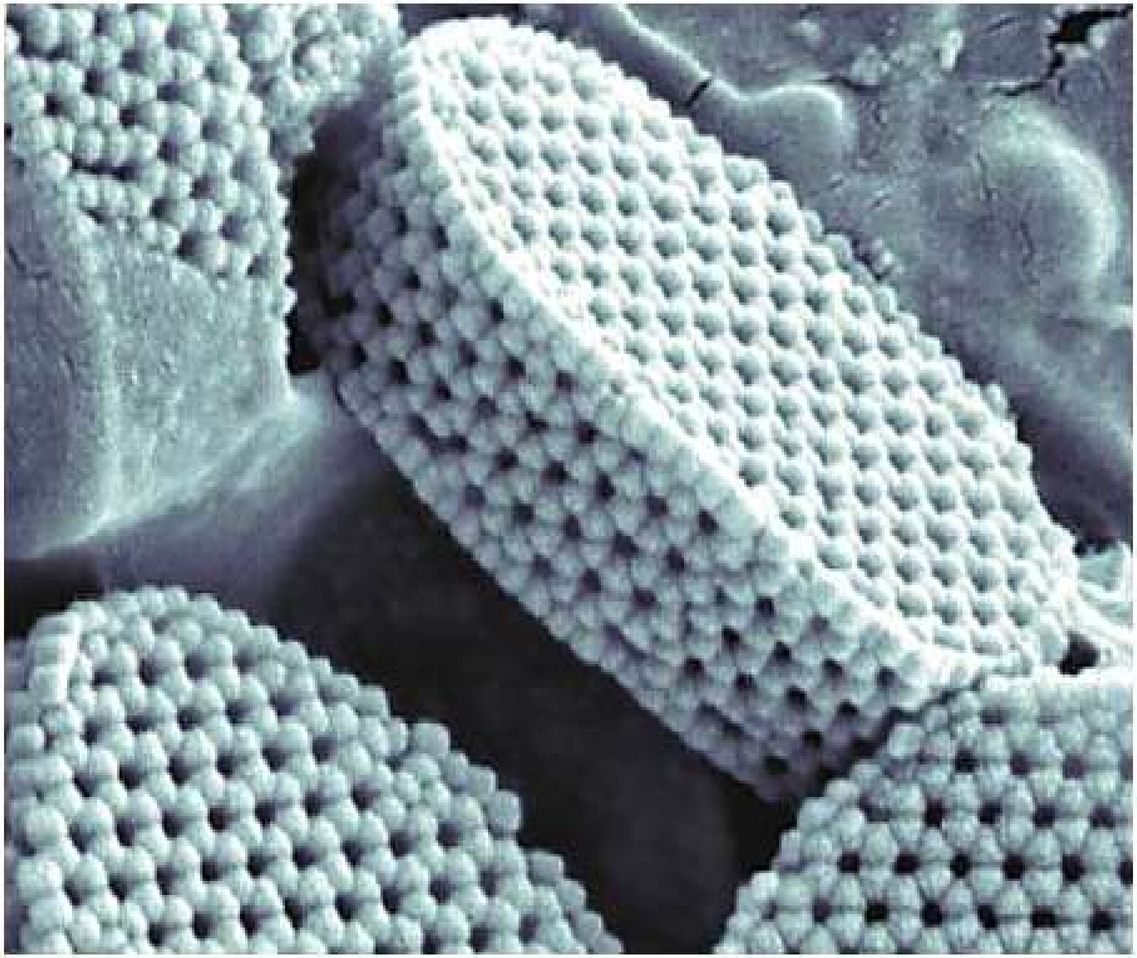
Diffraction causes gaps in the density of modes for *k* vectors near the planes in reciprocal space where diffraction occurs.





photon density of states for voids in an fcc lattice

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

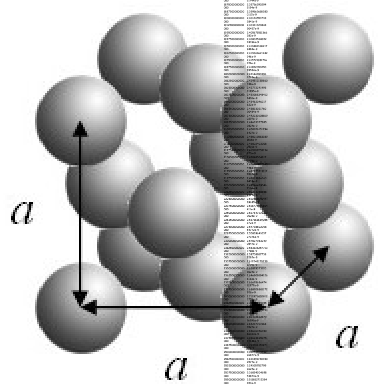


The alga Calyptrolithophora papillifera is encased in a shell of calcite crystals with a two-layer structure (visible on oblique face). Calculations show that this protective covering reflects ultraviolet light. Image Credit: J. Young/Natural History Museum, London

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

Spheres on any 3-D Bravais lattice

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



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

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

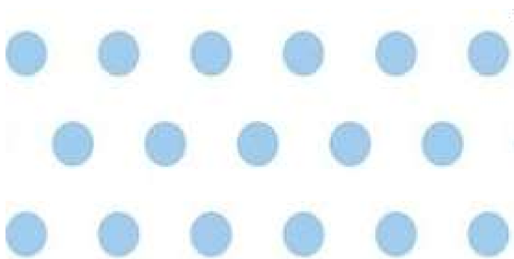
Central equations: $$\sum_{\vec{G}}\left(\vec{k}-\vec{G}\right)^2 b_{\vec{G}} A_{\vec{k}-\vec{G}} = \omega^2 A_{\vec{k}}$$

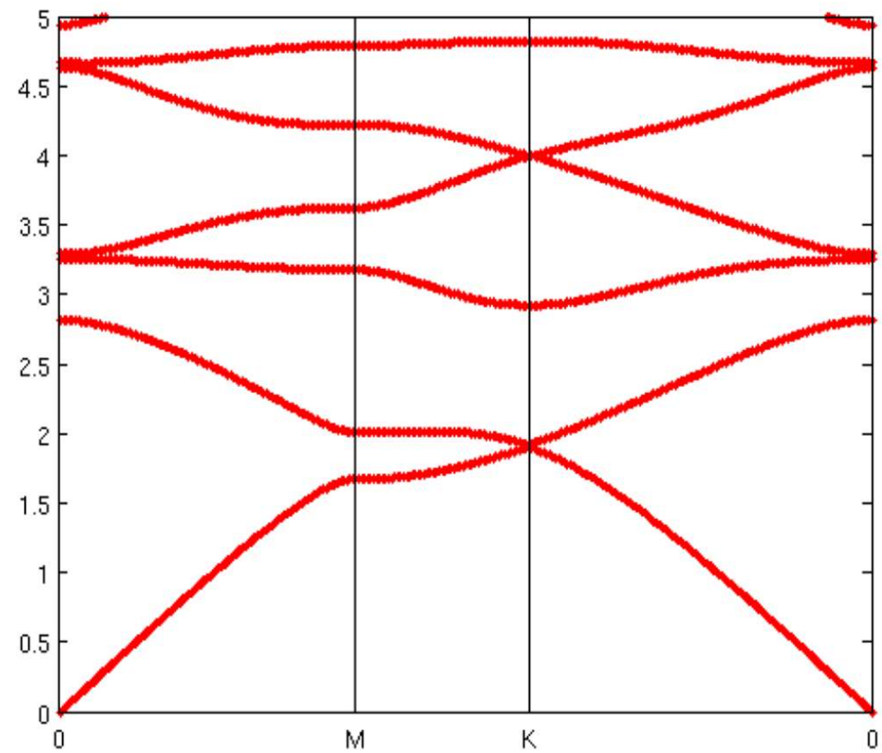
Choose a k value inside the 1st Brillouin zone. The coefficient A_k is coupled by the central equations to coefficients A_k outside the 1st Brillouin zone. Write these coupled equations in matrix form.

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

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

Close packed circles in 2-D





Solved by a student with the plane wave method