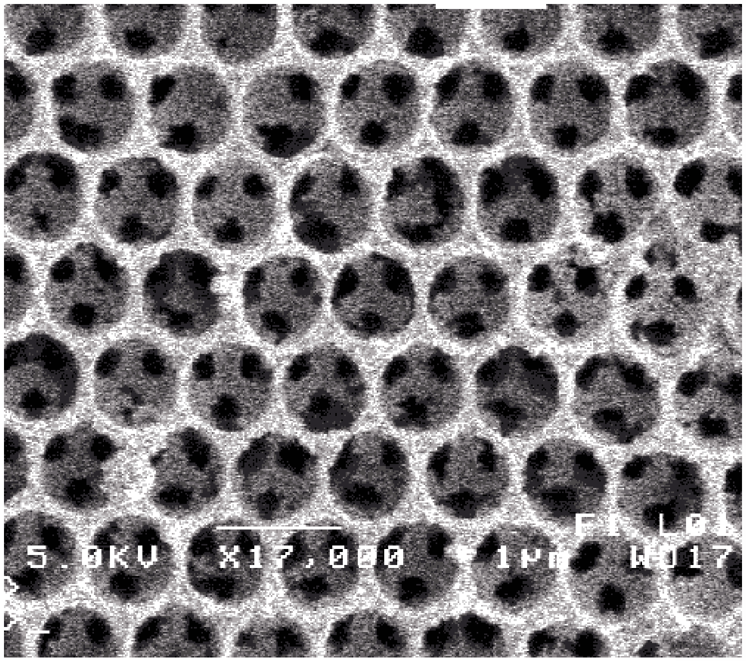
Technische Universität Graz

14. Photons

May 8, 2018

Inverse opal photonic crystal



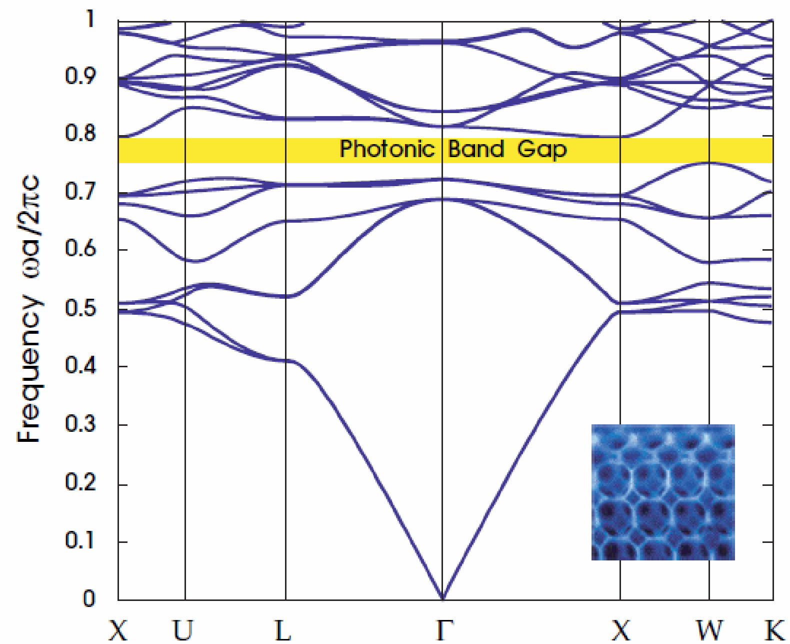
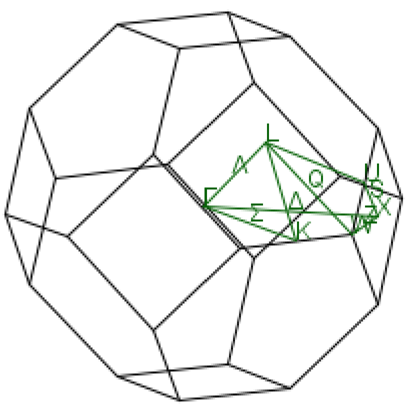


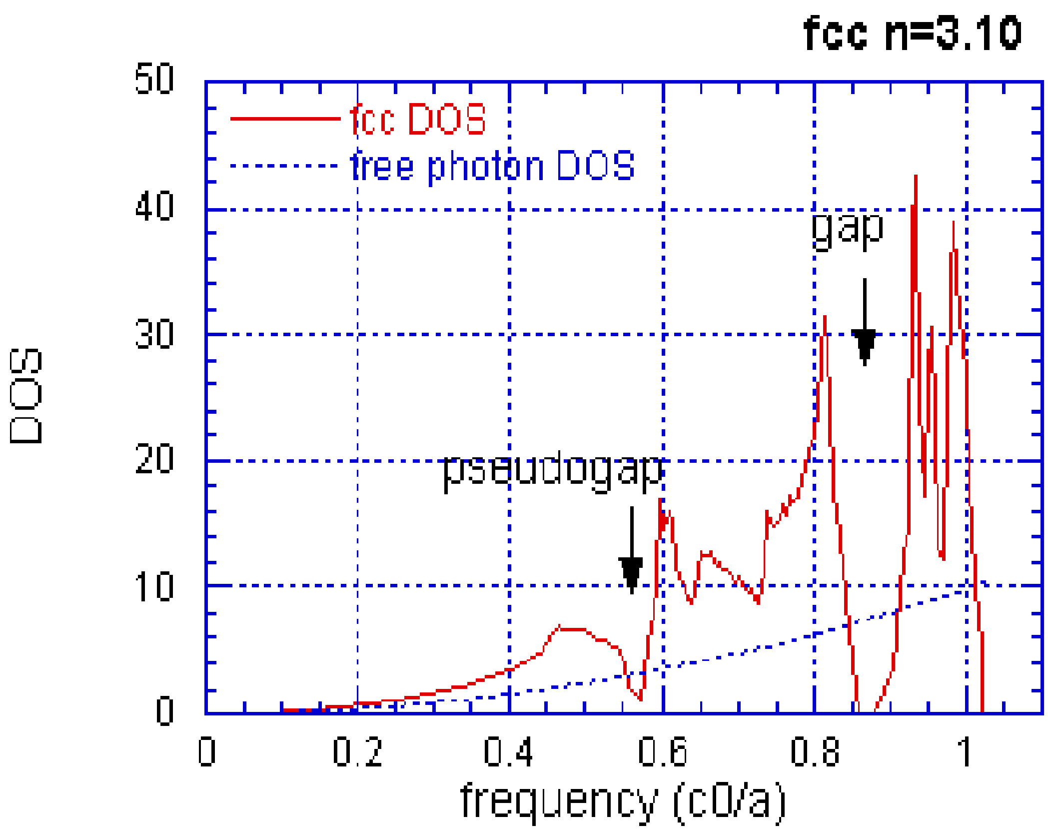
Figure 8: The photonic band structure for the lowest bands of an "inverse opal" structure: a face-centered cubic (fcc) lattice of close-packed air spheres in dielectric ($\varepsilon = 13$). (Inset shows fabricated structure from figure 9.) There is a complete photonic band gap (yellow) between the eighth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

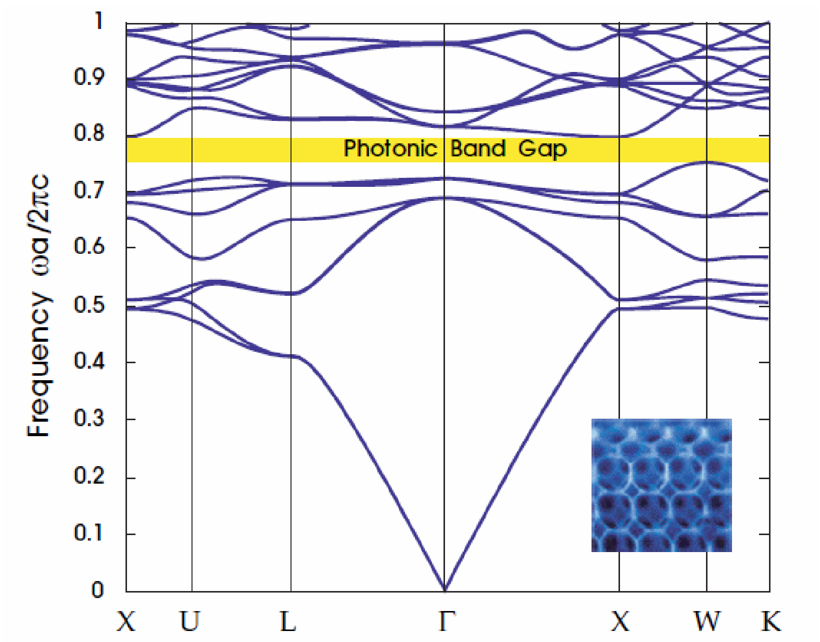


http://ab-initio.mit.edu/book

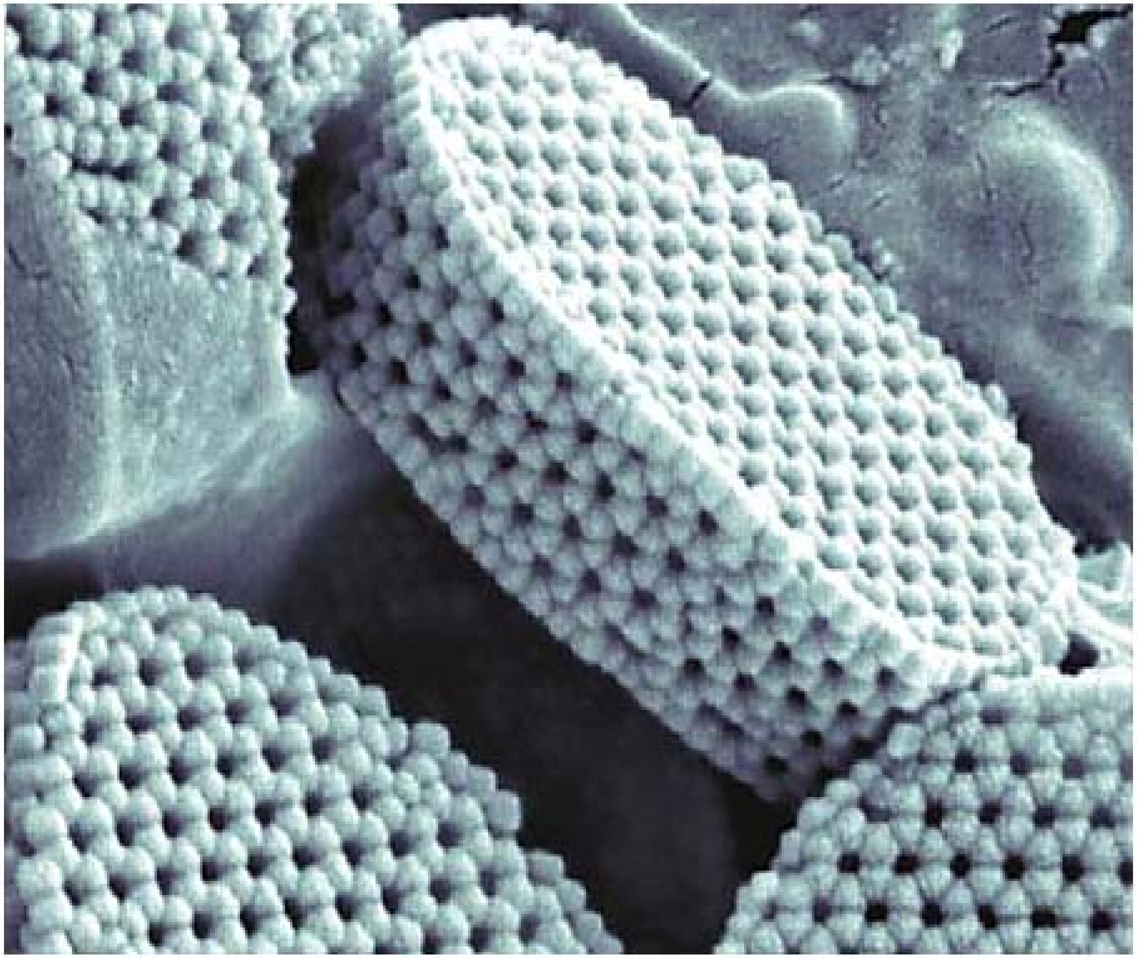
Photon density of states

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





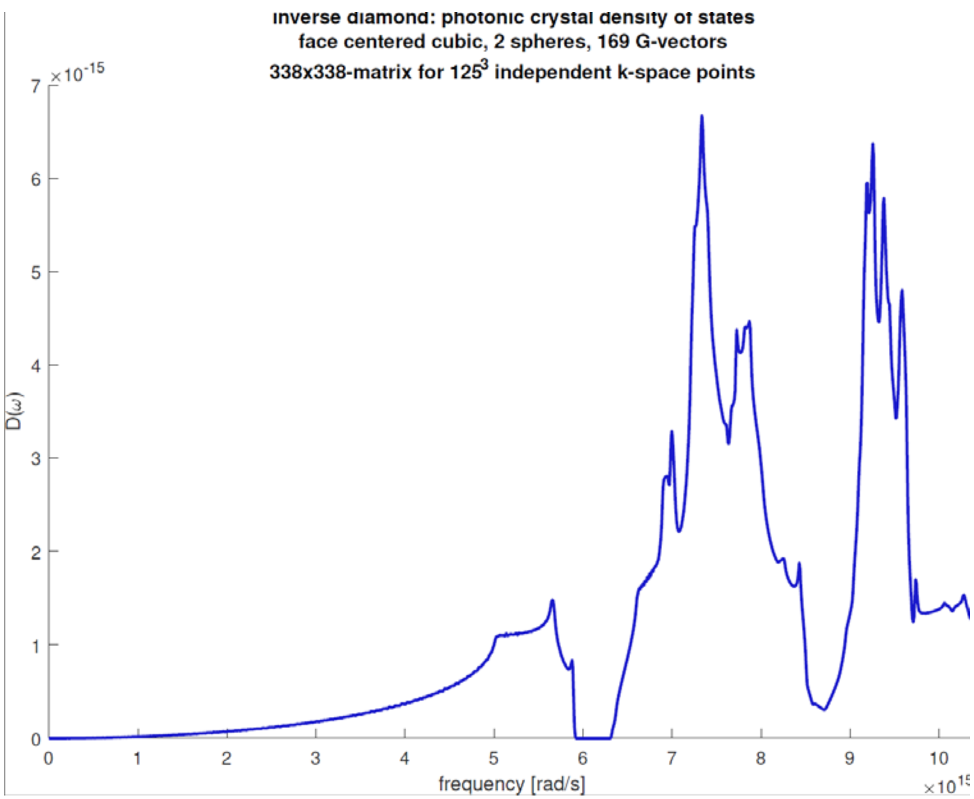
photon density of states for voids in an fcc lattice
http://www.public.iastate.edu/~cmpexp/groups/PBG/pres_mit_short/sld002.htm

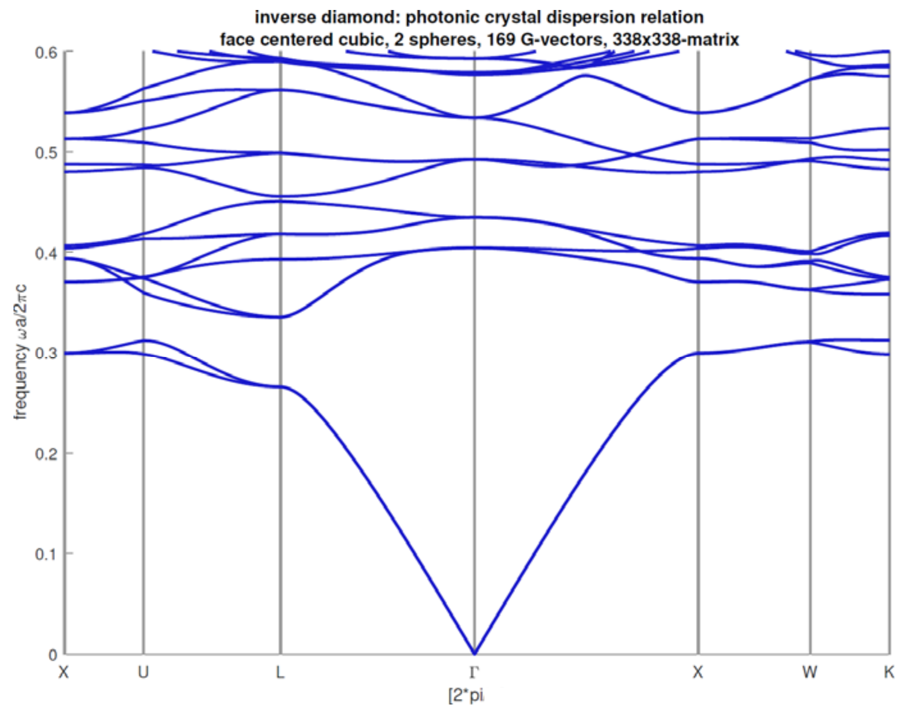


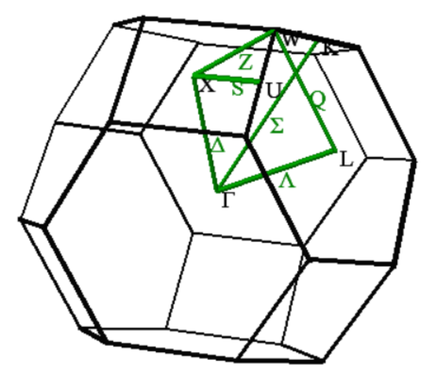
The alga Calyptrolithophora papillifera is encased in a shell of calcite crystals with a two-layer structure (visible on oblique face). Calculations show that this protective covering reflects ultraviolet light. Image Credit: J. Young/Natural History Museum, London

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

Inverse diamond



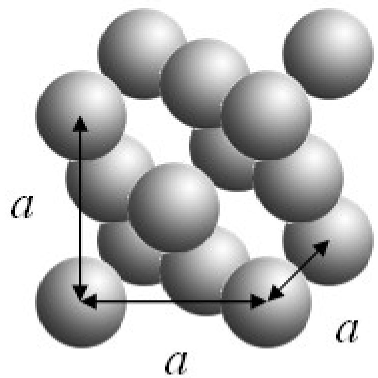




Solved by a student with the plane wave method

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

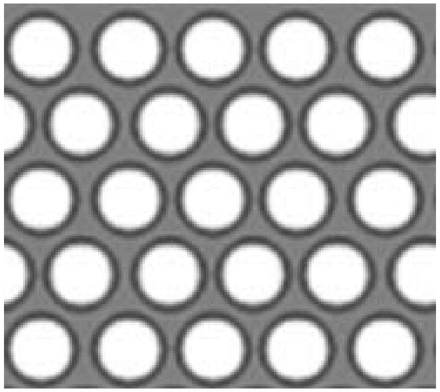
Central equations: $$\sum_{\vec{G}}\left(\vec{k}-\vec{G}\right)^2 b_{\vec{G}} A_{\vec{k}-\vec{G}} = \omega^2 A_{\vec{k}}$$

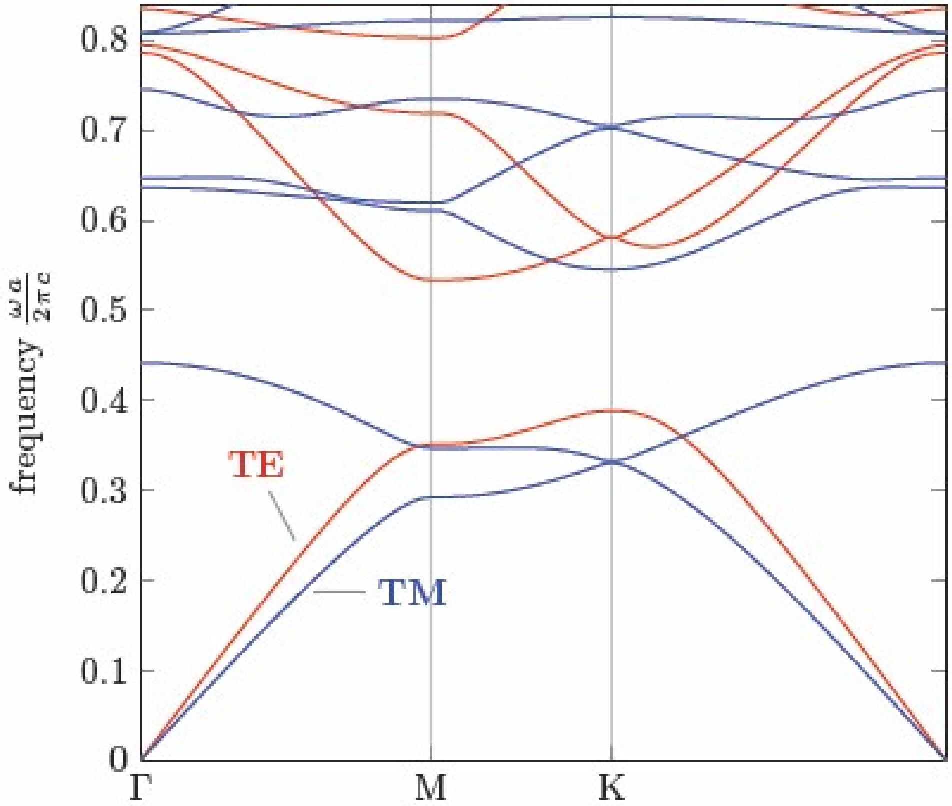
Choose a k value inside the 1st Brillouin zone. The coefficient A_k is coupled by the central equations to coefficients A_k outside the 1st Brillouin zone. Write these coupled equations in matrix form.

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

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

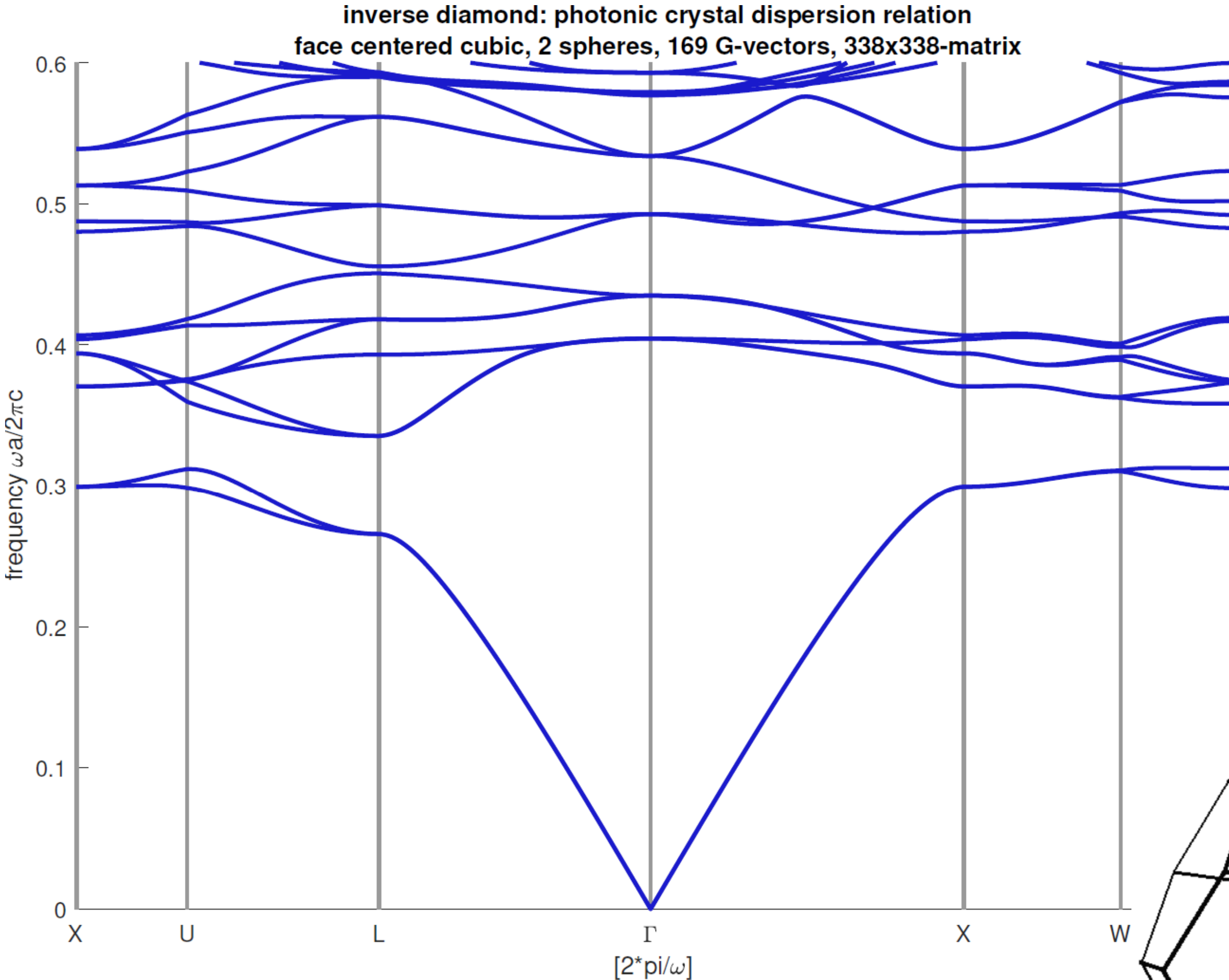
2-D array of air holes

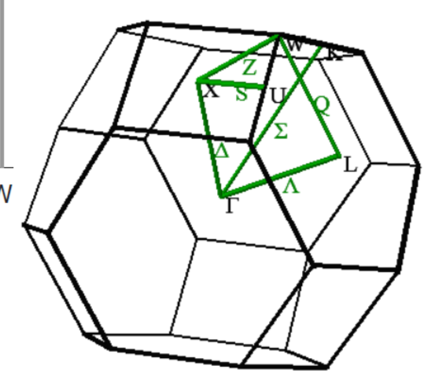




Solved by a student with the plane wave method

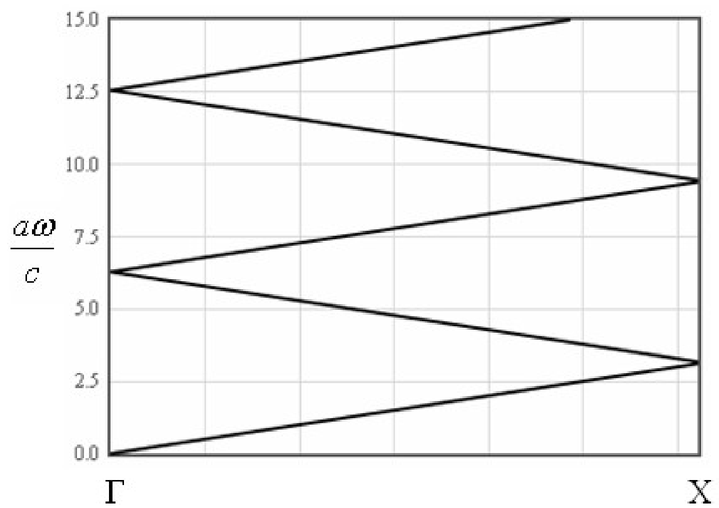
Inverse diamond

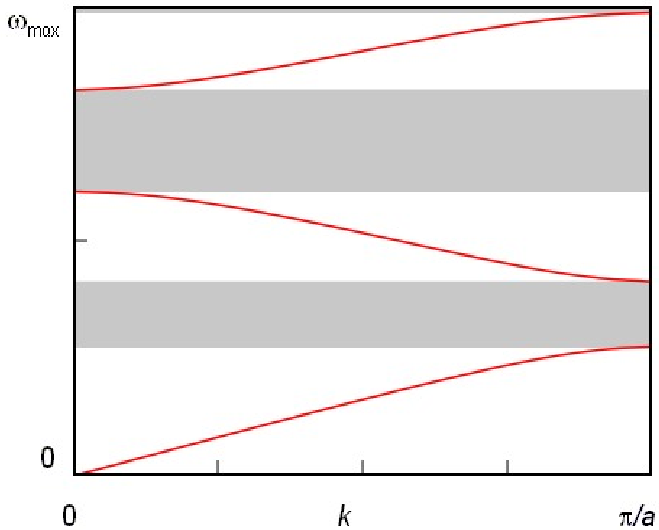


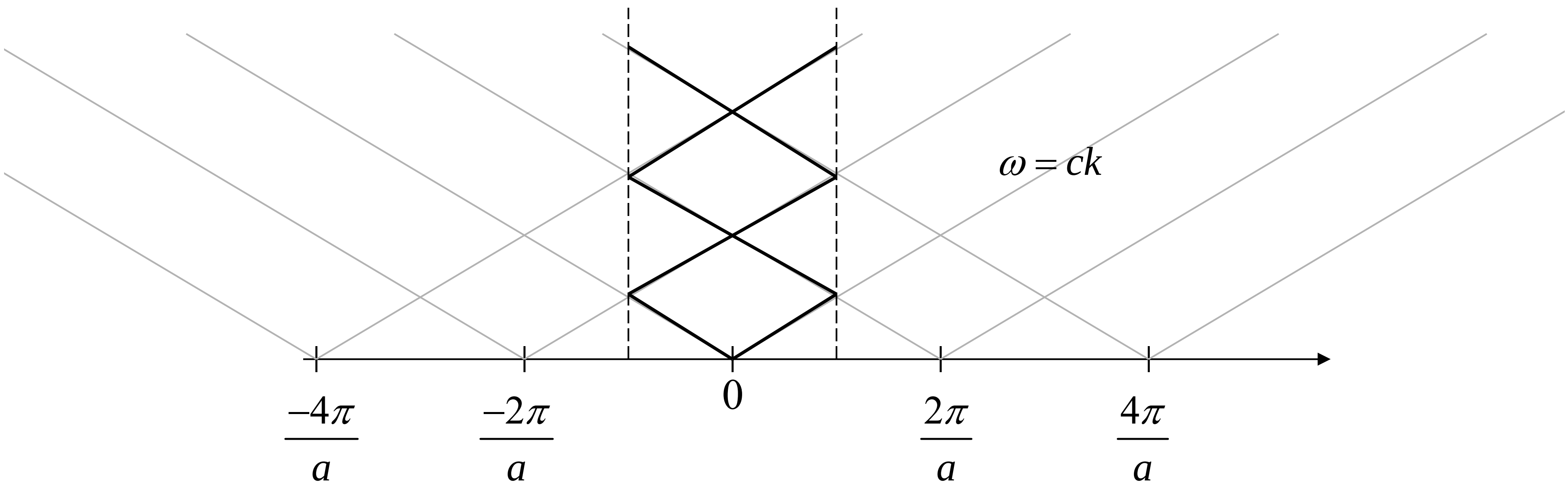


Solved by a student with the plane wave method

Empty lattice approximation

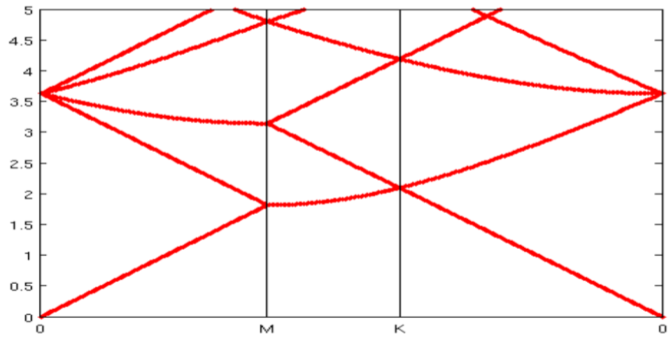


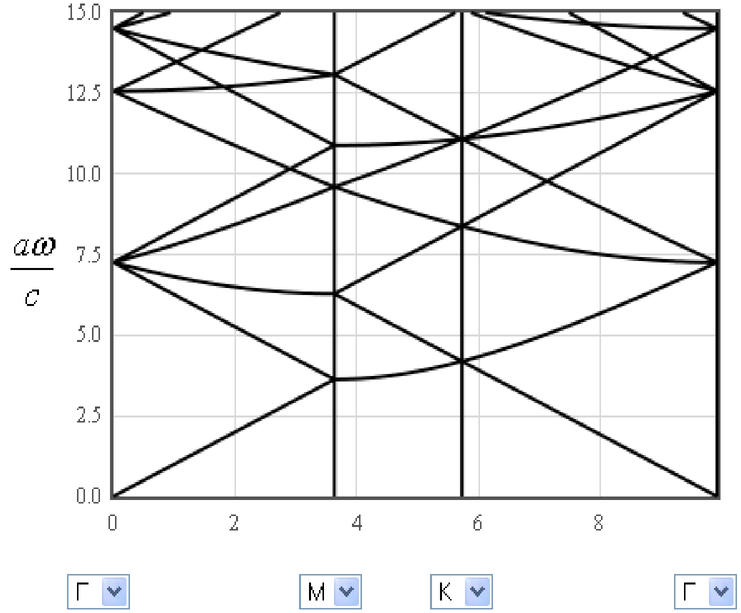


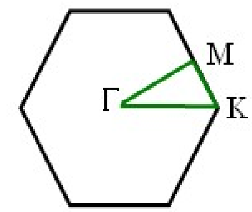


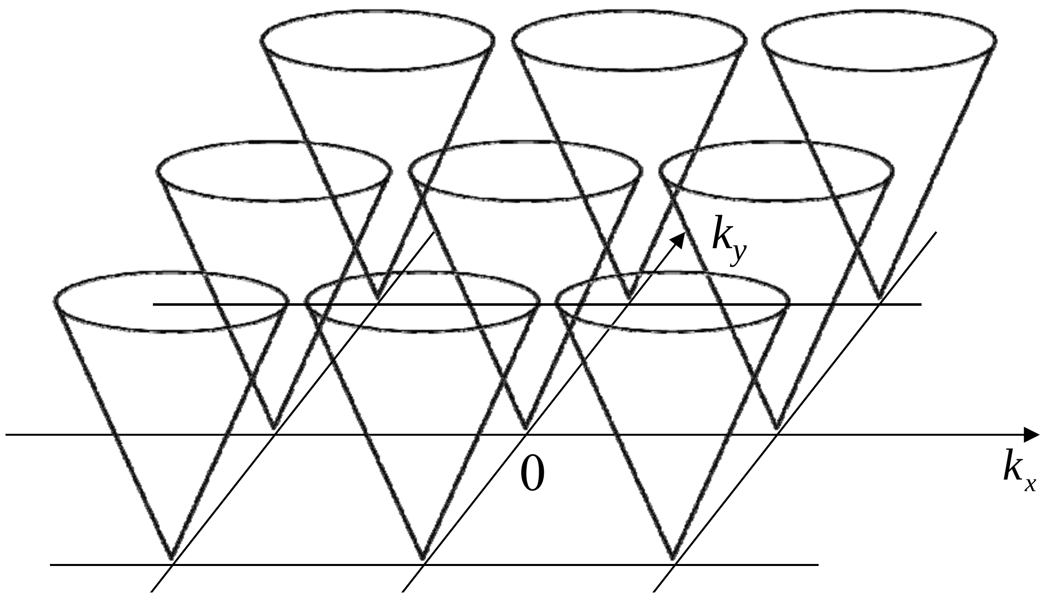
Empty lattice approximation

Plane wave method



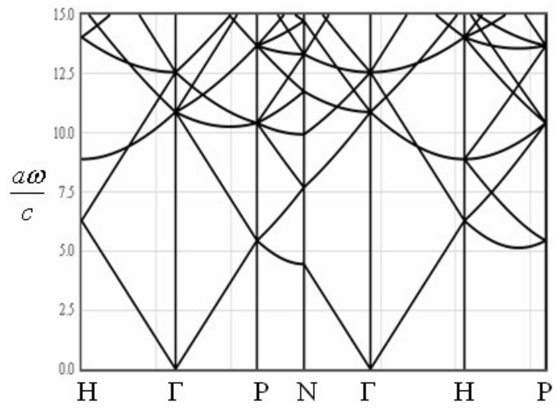




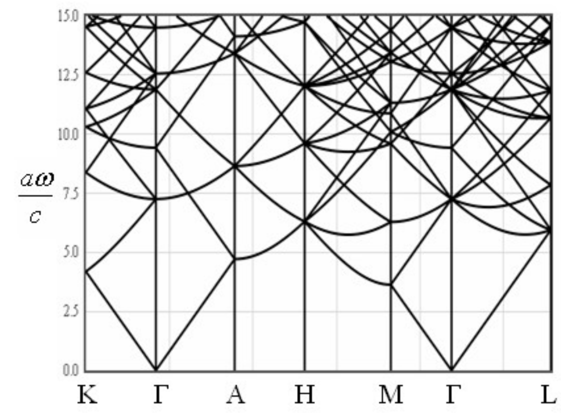


Empty lattice approximation

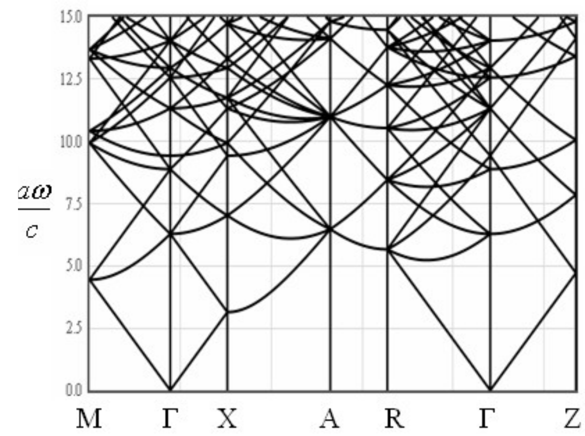
Body centered cubic

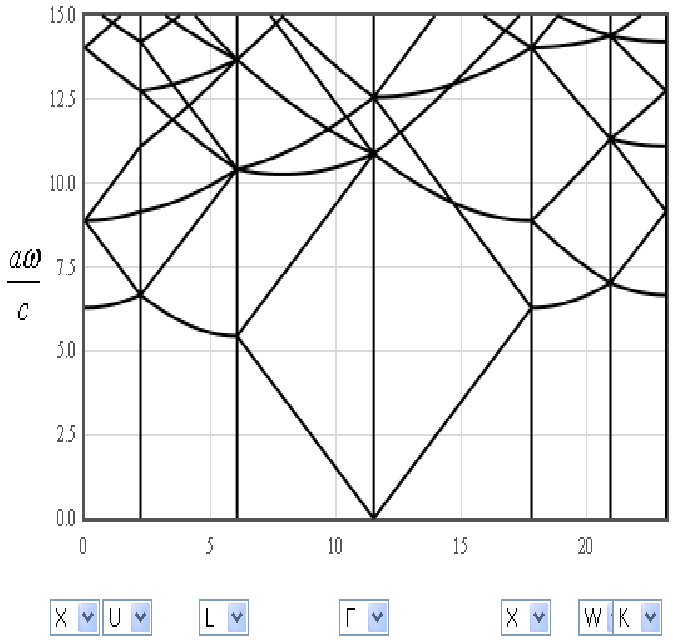


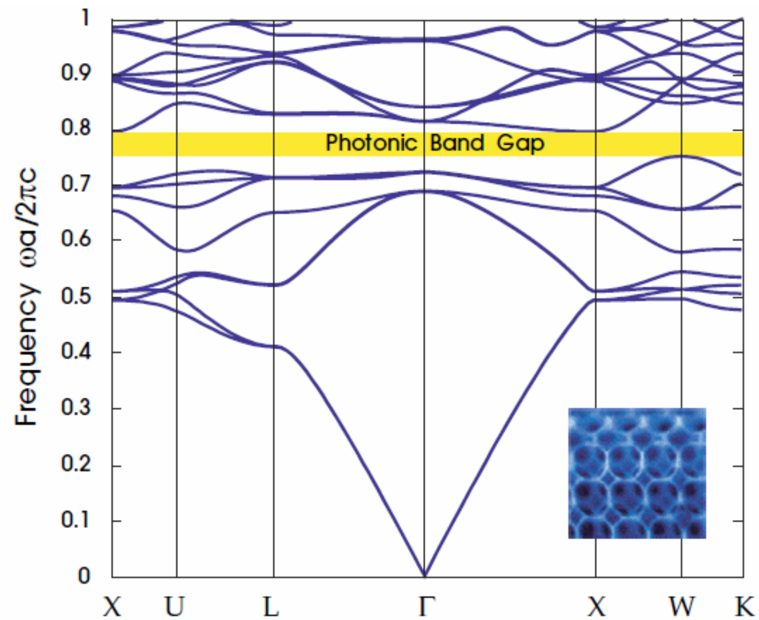
Hexagonal



Tetragonal







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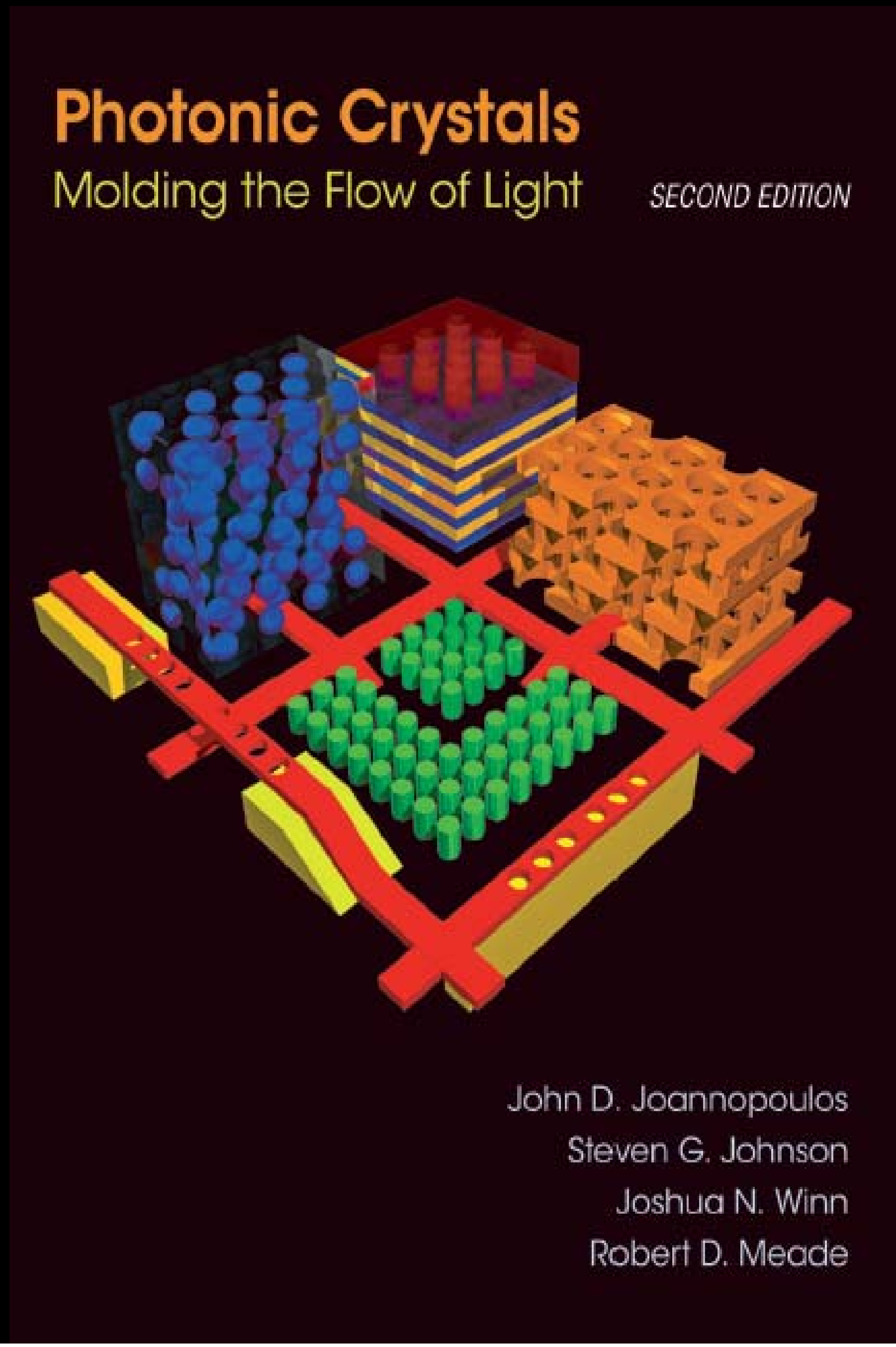
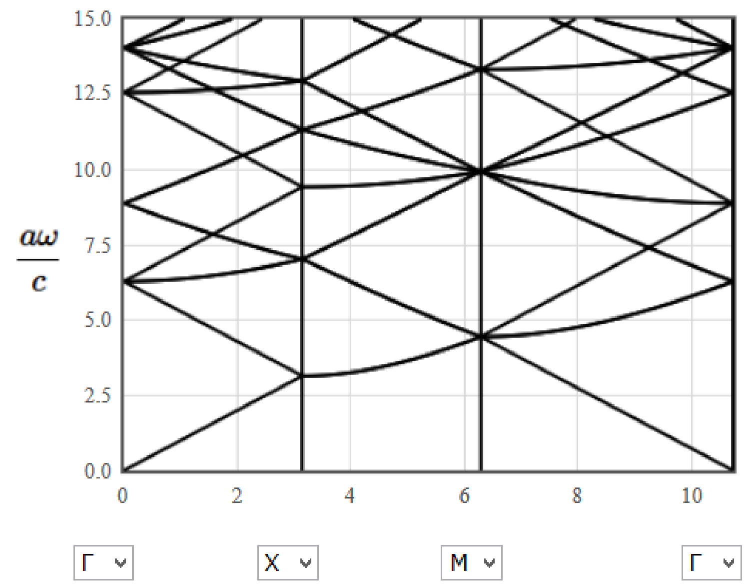
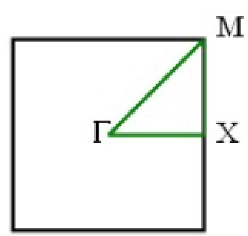
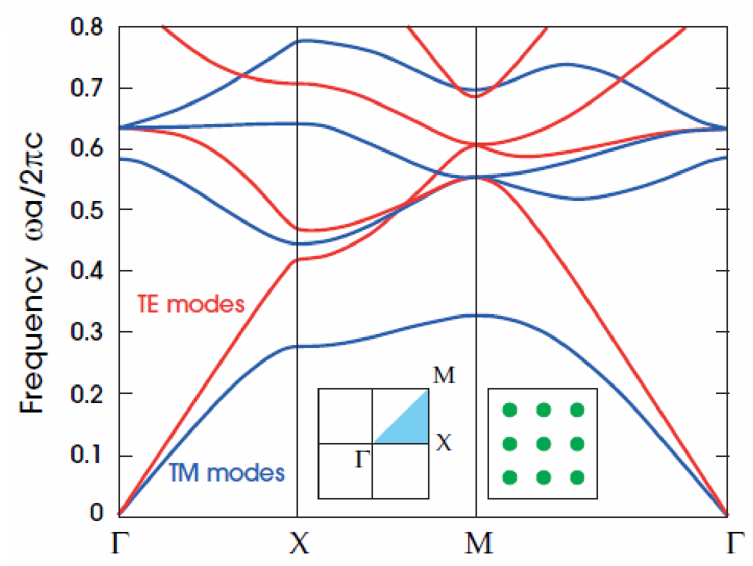


Empty lattice approximation







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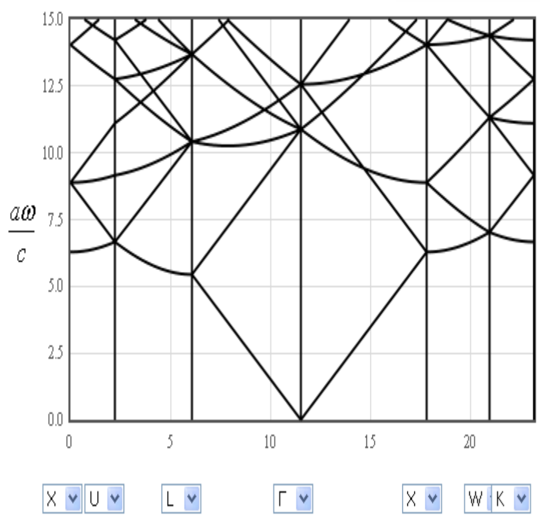
fcc



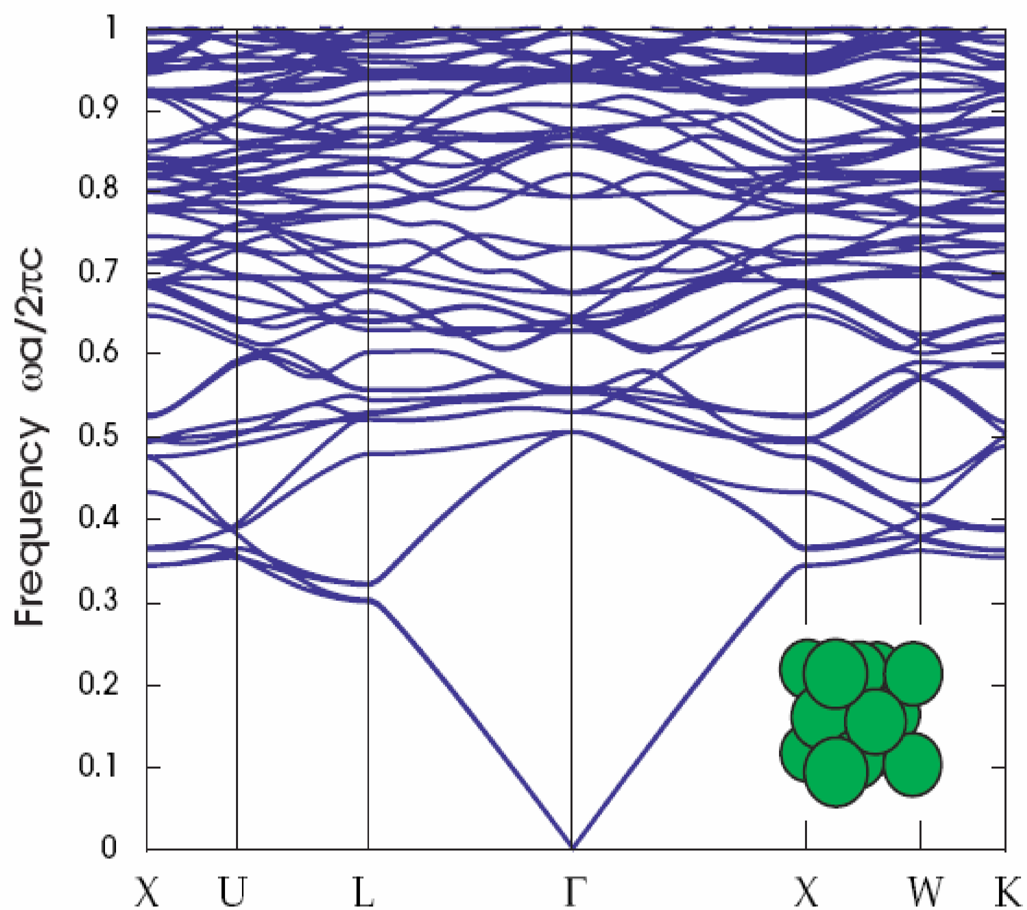


Figure 2: The photonic band structure for the lowest-frequency electromagnetic modes of a face-centered cubic (fcc) lattice of close-packed dielectric spheres ($\varepsilon = 13$) in air (inset). Note the *absence* of a complete photonic band gap. The wave vector varies across the irreducible Brillouin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

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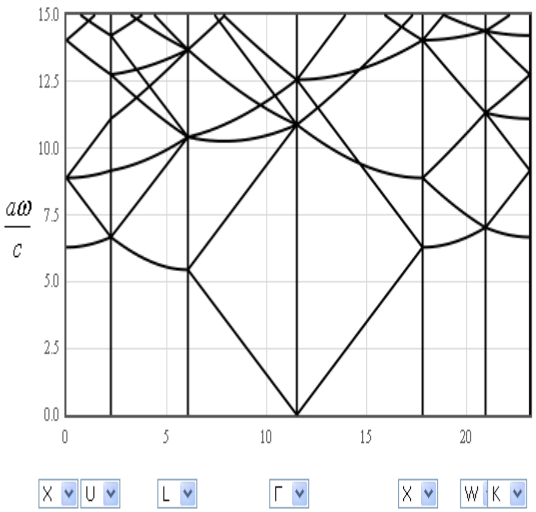
diamond



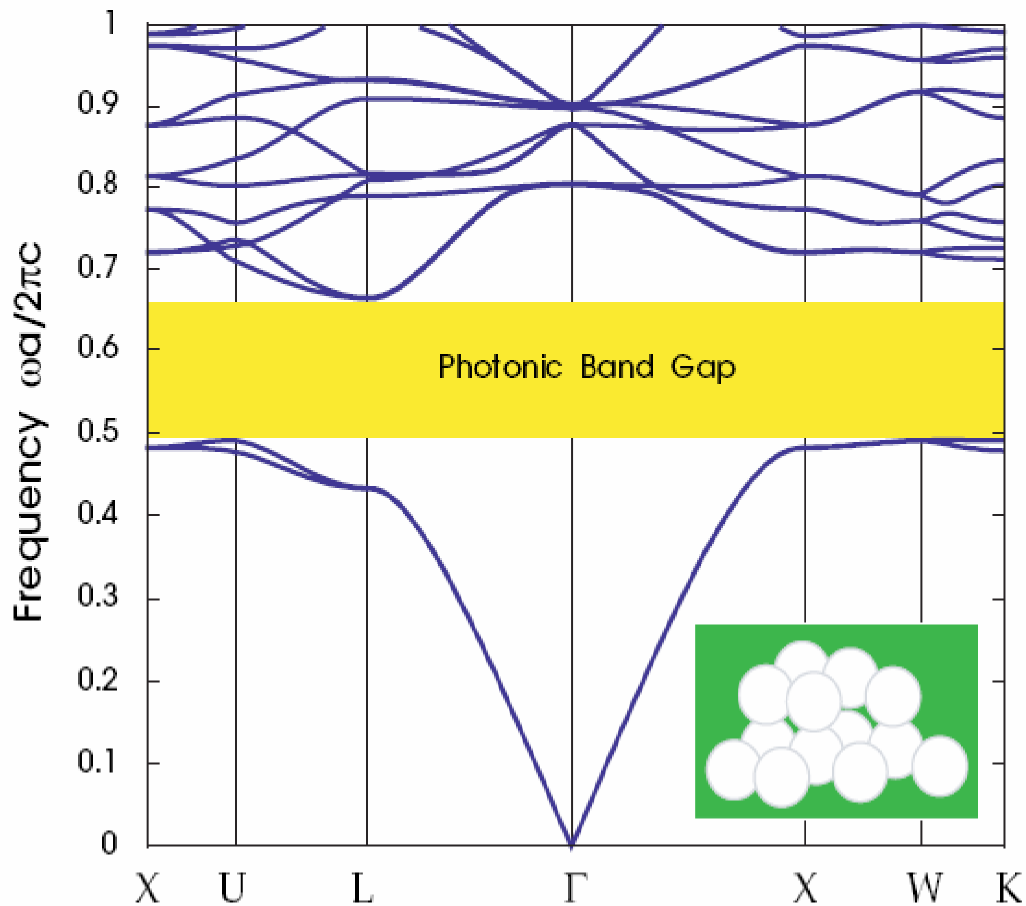


Figure 3: The photonic band structure for the lowest bands of a diamond lattice of air spheres in a high dielectric ($\varepsilon = 13$) material (inset). A complete photonic band gap is shown in yellow. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points;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

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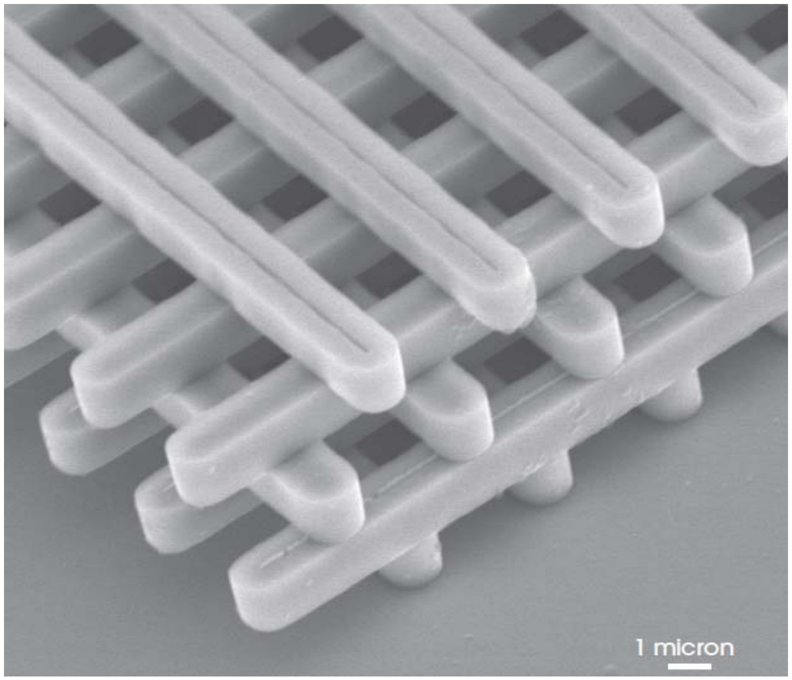
Woodpile photonic crystal



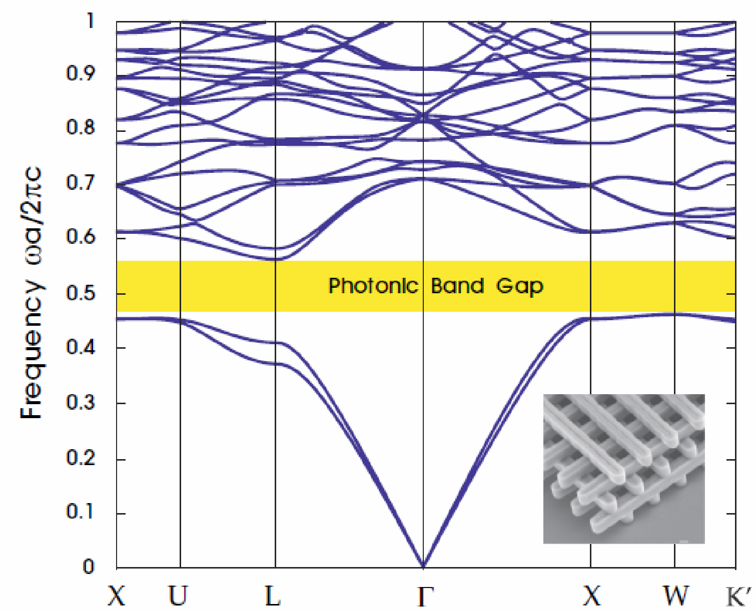
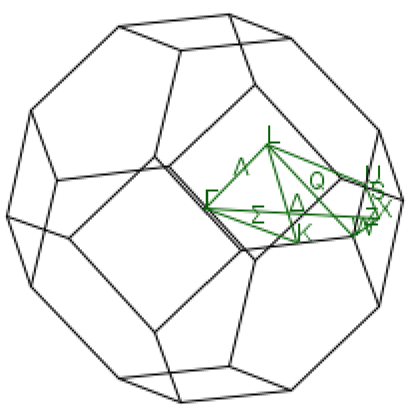


Figure 7: The photonic band structure for the lowest bands of the woodpile structure (inset, from figure 6) with $\varepsilon = 13$ logs in air. The irreducible Brillouin zone is larger than that of the fcc lattice described in appendix B, because of reduced symmetry—only a portion is shown, including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



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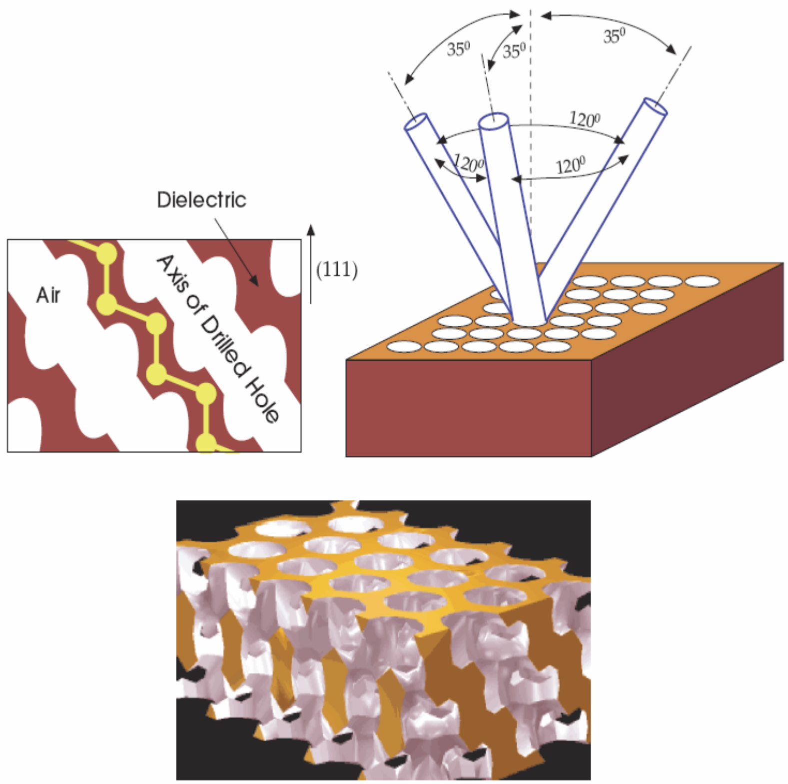
Yablonovite



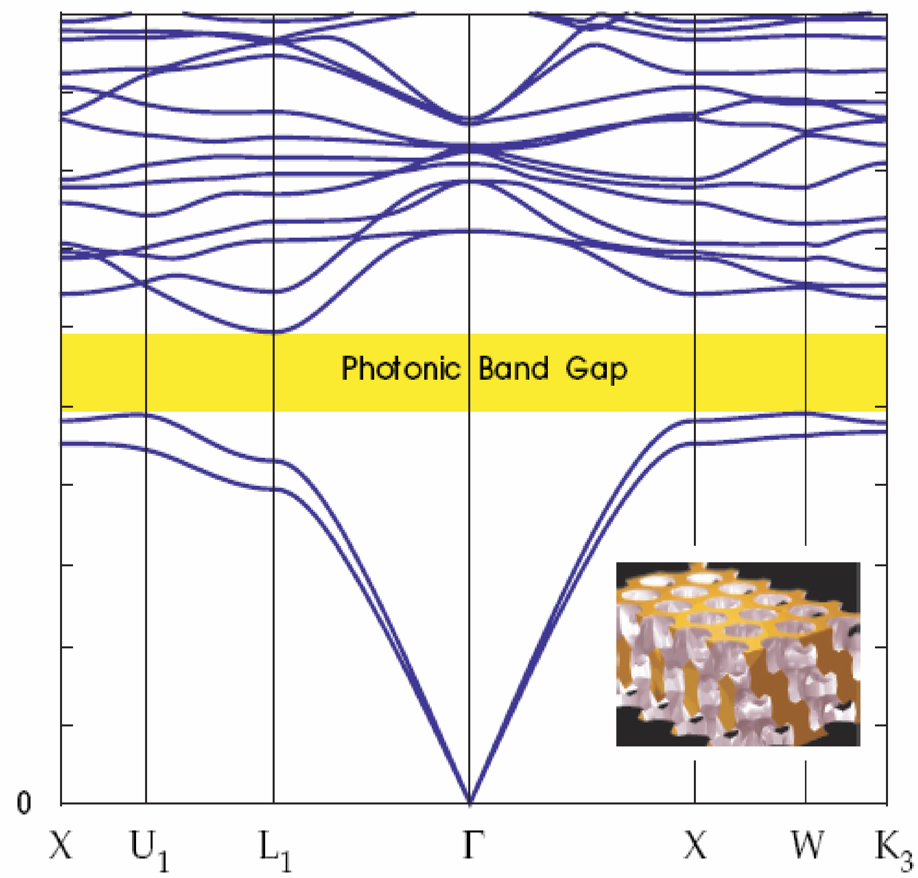


Figure 5: The photonic band structure for the lowest bands of Yablonovite (inset, from figure 4). Wave vectors are shown for a portion of the irreducible Brillouin zone that includes the edges of the complete gap (yellow). A detailed discussion of this band structure can be found in Yablonovitch et al.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

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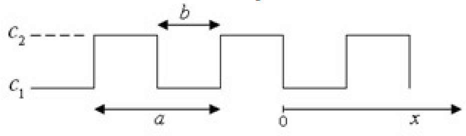
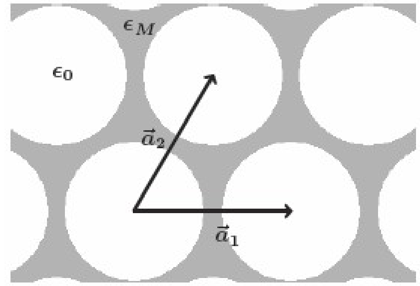
1-D Multilayer film

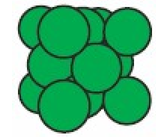


1-D Multilayer film

2-D triangular array of air holes



fcc



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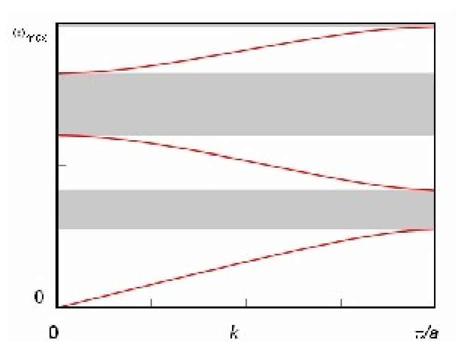
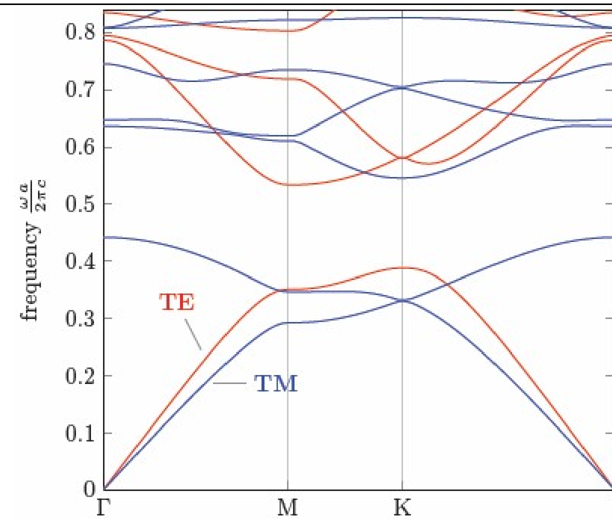
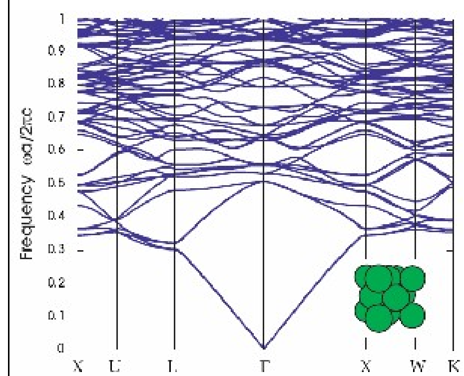


Calculate ω(k)





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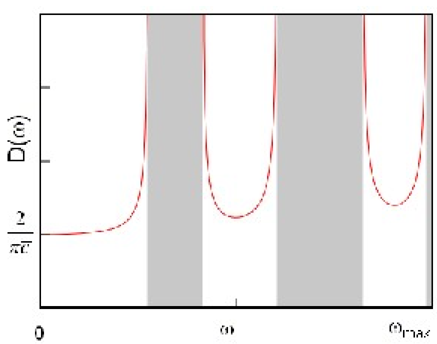
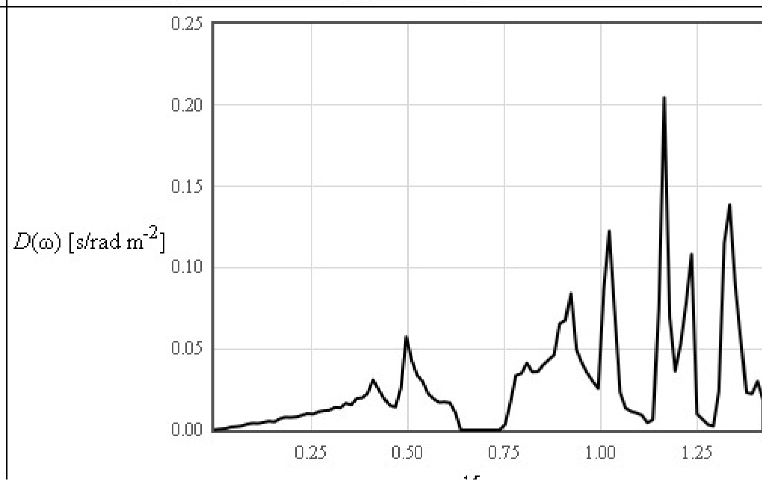


Calculate DoS



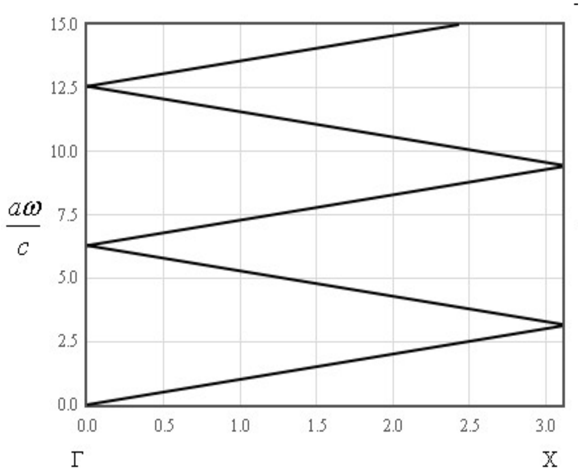
http://lampx.tugraz.at/~hadley/ss1/emfield/photonic_crystals/photonic_table.html

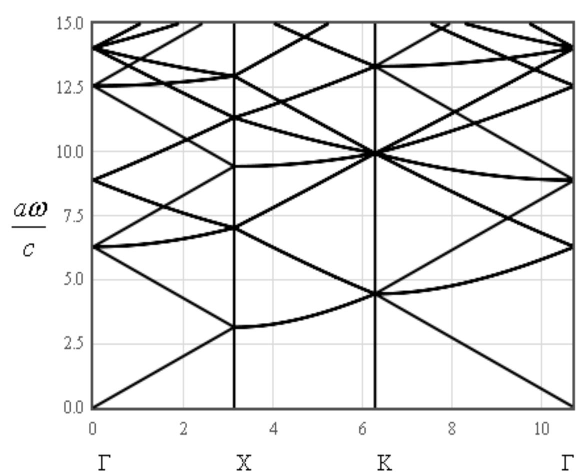
Student projects

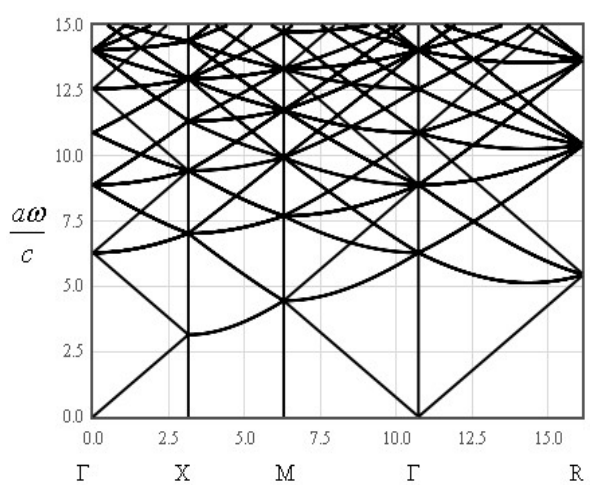
Use the plane wave method to calculate the dispersion relation for light in a 1-D layered material (or a 2-D or 3-D material)

Help complete the table of the empty lattice approximation

Adapt the program that solves the in 1-D Schroedinger equation to the wave equation





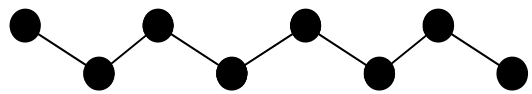


Lattice vibrations / Phonons

Phonons are quantum particles of sound

The simplest model for lattice vibrations is atoms connected by linear springs

There is a shortest wavelength/maximum frequency



Find the normal mode solutions

Quantize the normal modes

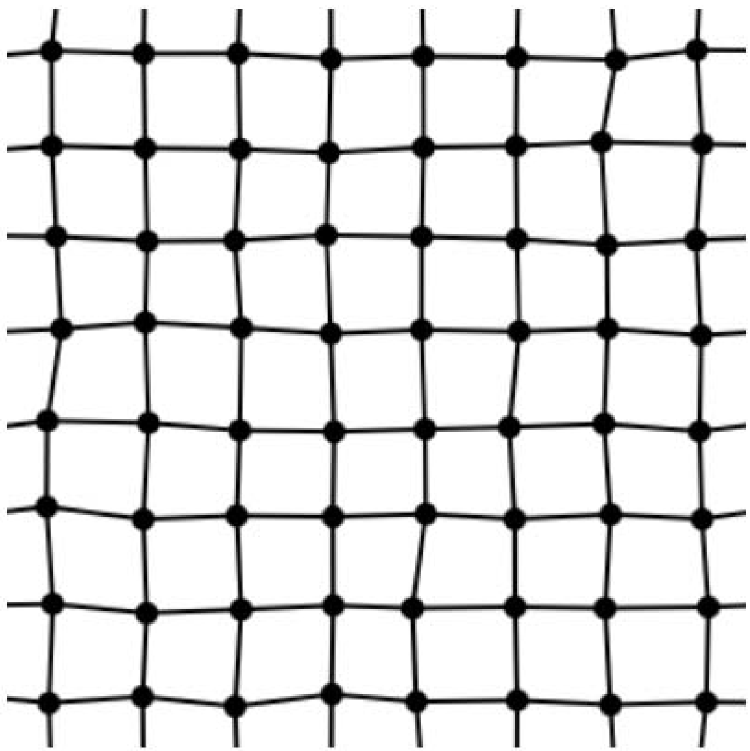
Find the phonon density of states

Calculate the thermodynamic properties

Menu | Sections | **PHY.F20 Molecular and Solid State Physics**

Normal Modes and Phonons

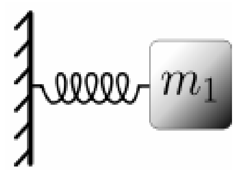
At finite temperatures, the atoms in a crystal vibrate. In the simulation below, the atoms move randomly around their equilibrium positions.



T = 300 K - +

http://lampx.tugraz.at/~hadley/ss1/phonons/phonon_script.php

Vibrations of a mass on a spring



$$m\frac{d^2x}{dt^2} = -Cx$$

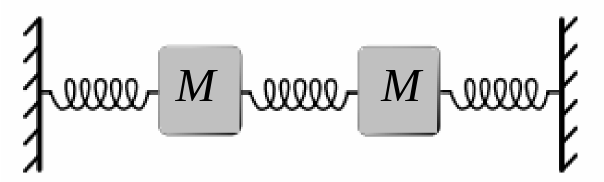
The solution has the form

$$x = A\mathrm{e}^{-i\omega t}$$

$$-\omega^2 mAe^{-i\omega t} = -CAe^{-i\omega t}$$

$$\omega = \sqrt{\frac{C}{m}}$$

Coupled masses



Newton's law

$$M\frac{d^2x_1}{dt^2} = -Cx_1 + C\left(x_2 - x_1\right) \qquad M\frac{d^2x_2}{dt^2} = -Cx_2 + C\left(x_1 - x_2\right)$$

assume harmonic solutions

$$x_1(t) = A_1\exp(i\omega t) \qquad x_2(t) = A_2\exp(i\omega t)$$

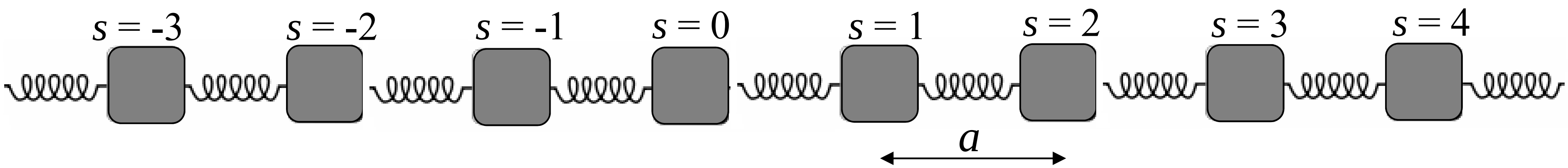
$$-\omega^2 MA_1e^{i\omega t} = -2CA_1e^{i\omega t} + CA_2e^{i\omega t}$$
$$-\omega^2 MA_2e^{i\omega t} = -2CA_2e^{i\omega t} + CA_1e^{i\omega t}$$

$$-\omega^2 M\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} -2C & C \\ C & -2C \end{bmatrix}\begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$$

Find the eigenvectors of this matrix

The masses oscillate with the same frequency but different phases

Linear Chain



$$m\frac{d^2u_s}{dt^2} = C(u_{s+1} - u_s) - C(u_s - u_{s-1}) = C(u_{s+1} - 2u_s + u_{s-1})$$

Assume every atom oscillates with the same frequency $u_s = A_s e^{-i\omega t}$

$$\begin{bmatrix} 2C-\omega^2 m & -C & 0 & 0 & 0 & -C \\ -C & 2C-\omega^2 m & -C & 0 & 0 & 0 \\ 0 & -C & 2C-\omega^2 m & -C & 0 & 0 \\ 0 & 0 & -C & 2C-\omega^2 m & -C & 0 \\ 0 & 0 & 0 & -C & 2C-\omega^2 m & -C \\ -C & 0 & 0 & 0 & -C & 2C-\omega^2 m \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \\ A_6 \end{bmatrix} = 0$$

$$\left[\left(2C - \omega^2 m\right)\mathrm{I} - C\left(\mathrm{T} + \mathrm{T}^{-1}\right)\right]\vec{A} = 0.$$

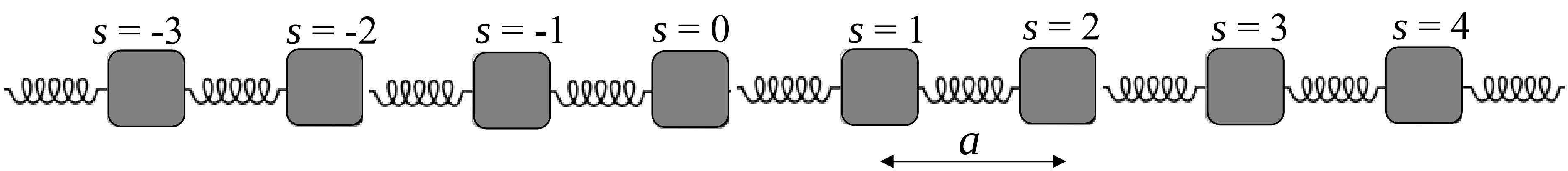
Eigen vectors of the translation operator

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ e^{i2\pi j/N} \\ e^{i4\pi j/N} \\ e^{i4\pi j/N} \\ \vdots \\ e^{i2\pi(N-1)j/N} \end{bmatrix} \quad j = 1, \cdots, N$$

$$\begin{bmatrix} 1 \\ e^{ika} \\ e^{i2ka} \\ e^{i3ka} \\ \vdots \\ e^{-ika} \end{bmatrix} \quad k = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \cdots$$

Linear Chain



solution: $u_s = A_k e^{i(ksa-\omega t)} = A_k e^{iksa} e^{-i\omega t}$