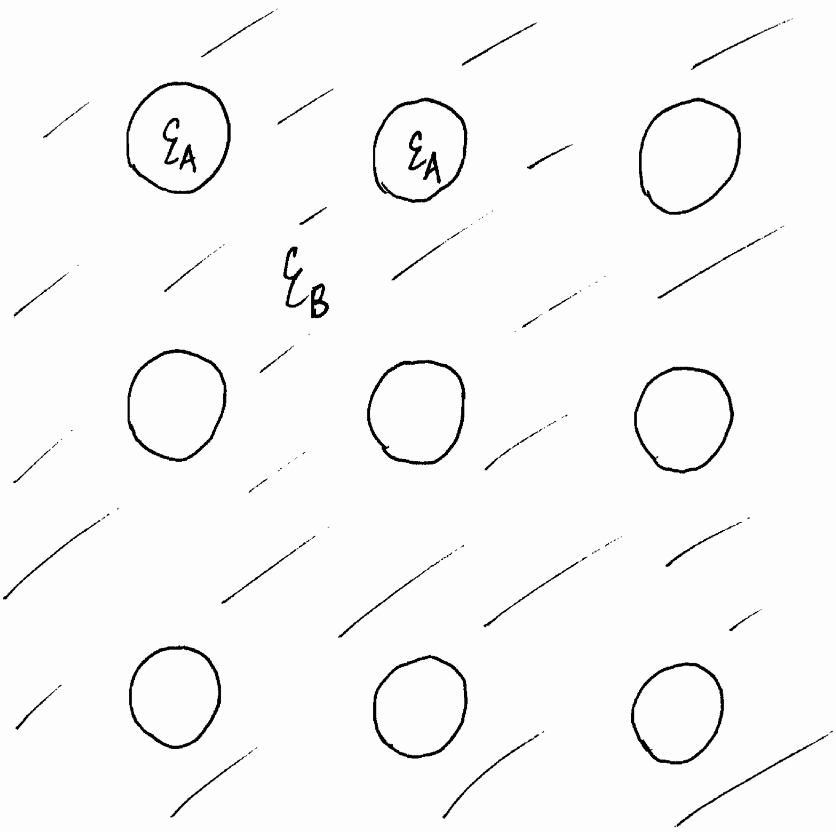
Photonic Crystals or Photonic Band Gap Materials

- Periodic array of a dielectric of ε_A in a host medium of dielectric ε_B
- Could be 3D [e.g. spheres of ε_A in host of ε_B]
  2D [e.g. cylinders of ε_A in host of ε_B]
  1D [e.g. a superlattices of ε_A and ε_B layers]

PGB materials usually refer to 2D and 3D structures.



Basic Wave Equations

- Maxwell's Equations
- Now, $\varepsilon(\vec{r})$ and possibly $\mu(\vec{r})$

$$\vec{\nabla} \times \frac{1}{\mu(\vec{r})} \vec{\nabla} \times \vec{E}(\vec{r},t) = -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \left(\varepsilon(\vec{r}) \vec{E}(\vec{r},t) \right)$$

and

$$\vec{\nabla} \times \frac{1}{\varepsilon(\vec{r})} \vec{\nabla} \times \vec{H}(\vec{r},t) = -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \left(\mu(\vec{r}) \vec{H}(\vec{r},t) \right)$$

(for sources outside region of interest)

[c.f.: Schrödinger Eq. (time dependent) in band problem and Newton's law in phonon problem.]

- Turn them into "time-independent" equations: Consider monochromatic wave of frequency ω with $e^{-i\omega t}$ time dependence:

$$\boxed{\begin{aligned} &\vec{\nabla} \times \frac{1}{\mu(\vec{r})} \vec{\nabla} \times \vec{E}(\vec{r}) - \frac{\omega^2}{c^2} \epsilon(\vec{r}) \vec{E}(\vec{r}) = 0 \\ &\vec{\nabla} \times \frac{1}{\varepsilon(\vec{r})} \vec{\nabla} \times \vec{H}(\vec{r}) - \frac{\omega^2}{c^2} \mu(\vec{r}) \vec{H}(\vec{r}) = 0 \end{aligned}}$$

- Typically, materials are non-magnetic. Thus, $\mu = 1$ everywhere†.

$$\boxed{\begin{array}{l} \text{The } \vec{E} \text{ and } \vec{H} \text{ equations become:} \\ \vec{\nabla} \times \vec{\nabla} \times \vec{E}(\vec{r}) - \frac{\omega^2}{c^2} \epsilon(\vec{r}) \vec{E}(\vec{r}) = 0 \quad (1) \\ \vec{\nabla} \times \frac{1}{\epsilon(\vec{r})} \vec{\nabla} \times \vec{H}(\vec{r}) - \frac{\omega^2}{c^2} \vec{H}(\vec{r}) = 0 \quad (2) \\ \text{with } \epsilon(\vec{r}) = \epsilon(\vec{r} + \vec{R}) \end{array}}$$

→ Starting point for photonic band structure calculations.

$$\left\{ \begin{array}{l} \underline{\text{c.f.}} \quad \frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r}) \\ \quad \text{with } V(\vec{r}) = V(\vec{r} + \vec{R}) \end{array} \right.$$

→ Starting point for electronic band structure calculations.

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† There are "meta-materials" that play with special-designed values of μ.

- Formally, one can turn Eq.(1) into an $\infty \times \infty$ matrix equation.

Note that:

$$\vec{E}_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\,\vec{u}_E(\vec{r}) \quad \text{periodic} \quad \text{(Bloch's theorem)}$$

$$= \sum_{\vec{G}} \vec{E}_{\vec{k}}(\vec{G})\, e^{i(\vec{k}+\vec{G})\cdot\vec{r}}$$

and

$$\begin{cases} \varepsilon(\vec{r}) = \sum_{\vec{G}} \varepsilon(\vec{G})\, e^{i\vec{G}\cdot\vec{r}} & (\because \varepsilon(\vec{r}) \text{ is periodic}) \\ \text{with } \varepsilon(\vec{G}) = \frac{1}{\Omega_c}\int_{\Omega_c} \varepsilon(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, d^3r \end{cases}$$

Eq. (1): $\vec{\nabla}\times\vec{\nabla}\times\vec{E}(\vec{r}) - \frac{\omega^2}{c^2}\varepsilon(\vec{r})\vec{E}(\vec{r}) = 0$

becomes

$$\boxed{(\vec{k}+\vec{G})\times\left[(\vec{k}+\vec{G})\times\vec{E}_{\vec{k}}(\vec{G})\right] + \frac{\omega^2}{c^2}\sum_{\vec{G}'}\varepsilon(\vec{G}-\vec{G}')\vec{E}_{\vec{k}}(\vec{G}') = 0 \qquad (1')}$$

- This is a matrix equation
- To solve for ω and the coefficients $\vec{E}_{\vec{k}}(\vec{G})$
- One equation for each $\vec{k}$
- $\vec{k} \in 1^{st}$ B.Z.

- Similarly, Eq. (2) can be turned into a matrix eqn.

Note that:

$$\vec{H}_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\,\vec{u}_H(\vec{r}) \quad \text{(Bloch's theorem)}$$

periodic

$$= \sum_{\vec{G}} \vec{H}_{\vec{k}}(\vec{G})\, e^{i(\vec{k}+\vec{G})\cdot\vec{r}}$$

$$\nu(\vec{r}) \equiv \frac{1}{\varepsilon(\vec{r})} = \sum_{\vec{G}} \nu(\vec{G})\, e^{i\vec{G}\cdot\vec{r}} \quad (\because \nu(\vec{r}) \text{ is periodic})$$

with $\nu(\vec{G}) = \frac{1}{\Omega_c}\int_{\Omega_c} \nu(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, d^3r$

Eq. (2): $\vec{\nabla} \times \left(\nu(\vec{r})\,\vec{\nabla} \times \vec{H}(\vec{r})\right) - \frac{\omega^2}{c^2}\vec{H}(\vec{r}) = 0$

becomes

$$\boxed{(\vec{k}+\vec{G}) \times \left[\sum_{\vec{G}'} \nu(\vec{G}-\vec{G}')\,(\vec{k}+\vec{G}') \times \vec{H}_{\vec{k}}(\vec{G}')\right] + \frac{\omega^2}{c^2}\vec{H}_{\vec{k}}(\vec{G}) = 0 \qquad (2')}$$

which is a matrix equation.

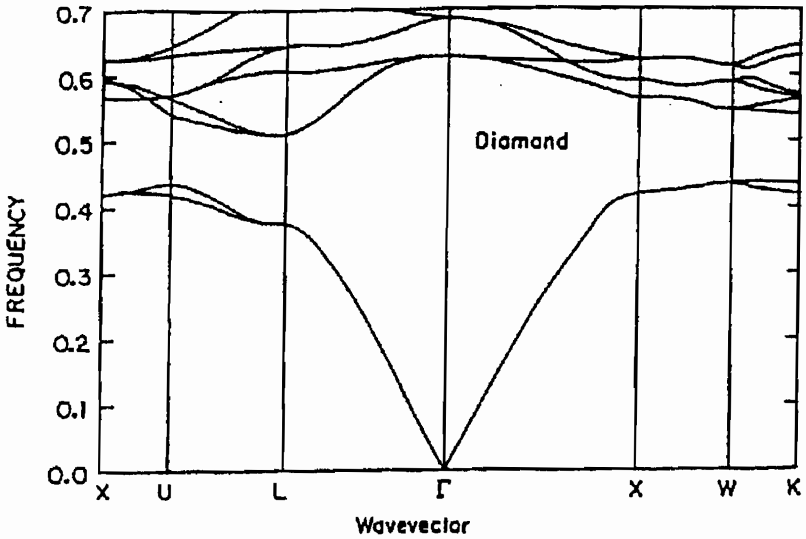
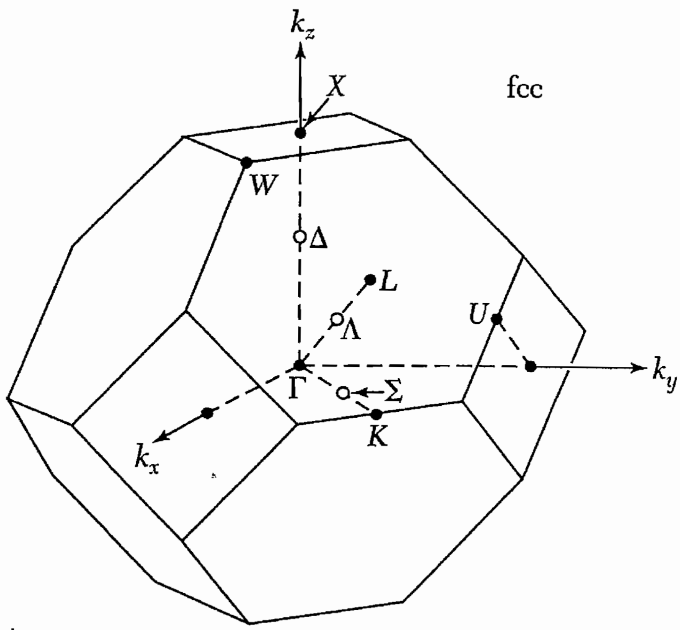


FIG. 3. Theoretical photonic band structure, calculated numerically using a plane- expansion, for a 3D diamond structure of dielectric spheres of refractive index 3.6 in an background. A filling fraction of 34% for the dielectric implies the spheres are just touc each other. A full photonic band gap appears between the second and third bands. Freque is in units of c/a where a is the lattice constant. [Taken from Fig. 2 of K. M. Ho, C. T. C and C. M. Soukoulis, *Phys. Rev. Lett.* 65, 3152 (1990).]



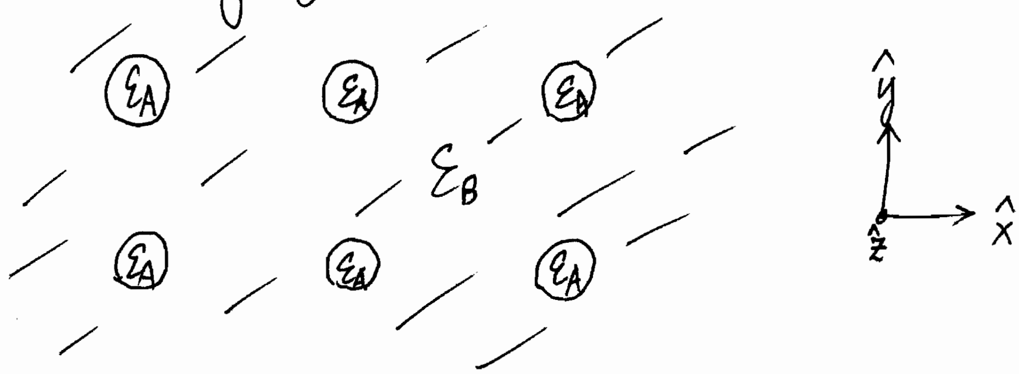
One can play with:

- Dielectric contrast, crystal structure, size of inclusions (filling fraction), shape of inclusion, basis in unit cell, dimensionality

- There are <u>special cases</u> where the equations (1) and (2) [or (1') and (2')] become simplier.

<u>Example</u>:

2D array of rods



Consider the special case of "TM modes"

$$\begin{cases} \vec{E} \parallel \hat{z} \ , & \vec{H} \text{ has } H_x, H_y \text{ components} \\ \varepsilon(x,y) \ , & \vec{k} = (k_x, k_y, 0) \in 1^{st} \text{ B.Z.} \end{cases}$$

$$\vec{E} = (0, 0, E_z(x,y)) \ ; \ \vec{H} = (H_x(x,y), H_y(x,y), 0)$$

In this case, the $\vec{E}$ equation becomes:

$$\boxed{\nabla^2 E_z(x,y) + \frac{\omega^2}{c^2}\epsilon(x,y)\, E_z(x,y) = 0}$$

∇^2: $\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$; $\epsilon(x,y)$: periodic

which is a standard scalar wave equation

→ easier to handle than vector fields

PBG B

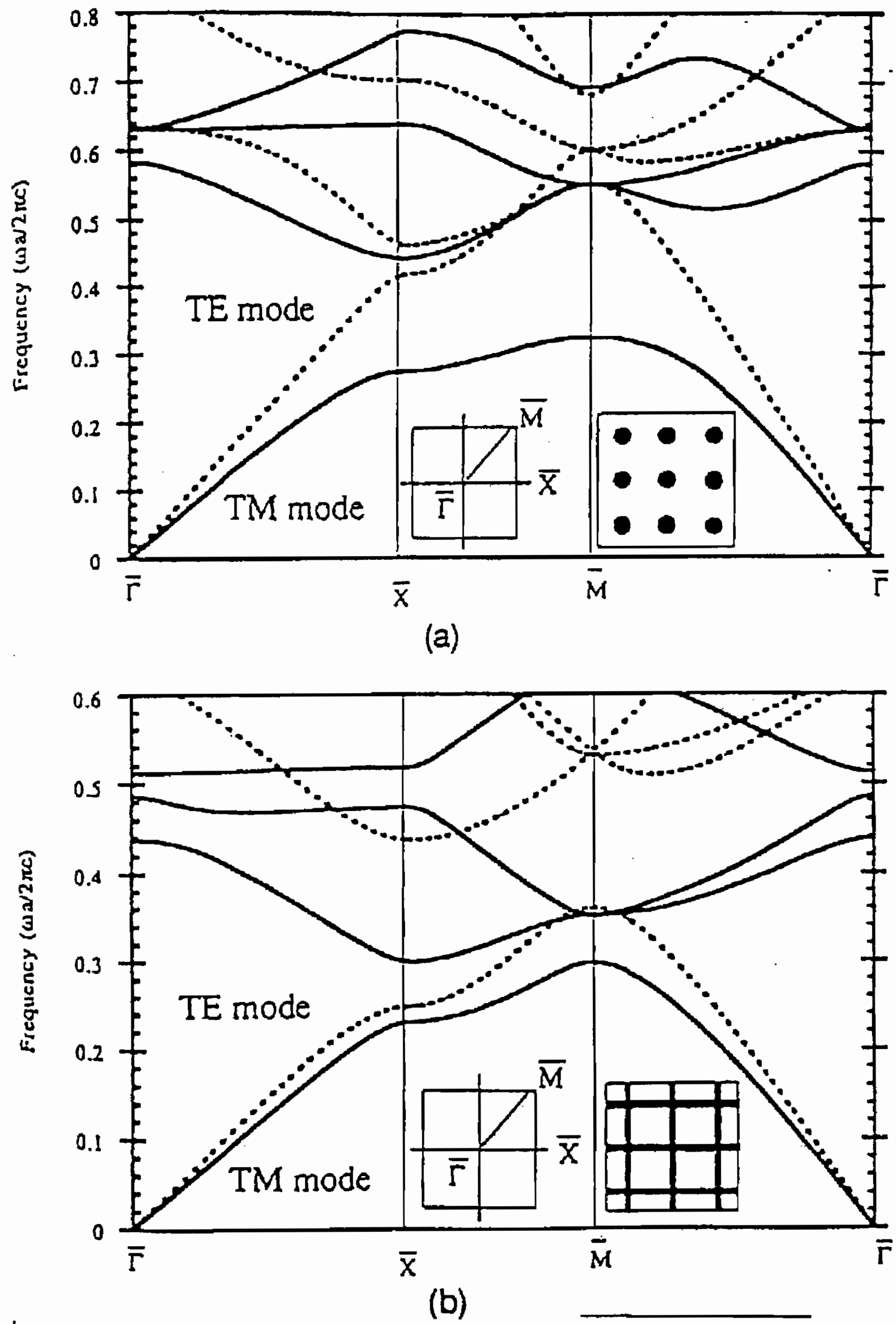


FIG. 5. Theoretical photonic band structure calculated numerically using a plane-wave expansion, for two 2D photonic (PBG) crystals. In (a) the PBG crystal is the same as that in Fig. 2. In (b) the PBG consists of a square array of square holes (side length $0.84a$) in a dielectric with $\epsilon = 8.9$. Cross sections of the crystals are shown in the insets. Solid lines represent TM modes [fields along (E_z, H_x, H_y)]; dashed lines represent TE modes [fields along (H_z, E_x, E_y)]. Brillouin zones are shown as insets. [Taken from Fig. 1 of R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos, *J. Opt. Soc. Am. B* 10, 328 (1993).]

Further Topics

- Structures for real gap (i.e., $\underline{k}$ in all directions)
- Applications
- Impurities
- Integration with other optical devices

References

- J. D. Joannopoulos, R. D. Meade, J. N. Winn "Photonic Crystals: Molding the Flow of Light" (Princeton University Press) [excellent introductory text]
- P. M. Hui and N. F. Johnson, "Photonic Band-Gap Materials", in Solid State Physics, Vol. 49, p. 151–203 (1995) (Academic Press). [more on band theoretical approaches]