ECE 595, Section 10
Numerical Simulations
Lecture 20: Bandstructure Concepts

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Outline

- Recap from Friday
- Bandstructure Problem Formulation
- Bloch's Theorem
- Reciprocal Lattice Space
- Numerical Solutions
  - 1D crystal
  - 2D triangular lattice
  - 3D diamond lattice

Recap from Friday: FEM for Electronic Transport

- Physics-based device modeling
- Electronic transport theory
- FEM electronic transport model
- Numerical results
- Error Analysis

Bandstructure Problem

- Amounts to solving an eigenvalue equation for a system with discrete translational symmetry
- Examples include:
  - Electronic bandstructure:
    $$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\Psi(x) = \hbar\omega\Psi(x)$$
  - Photonic bandstructure:
    $$\nabla \times [\epsilon^{-1}(\nabla \times H)] = \left(\frac{\omega}{c}\right)^2 H$$
  - Phononic bandstructure:
    $$\nabla \times [C(\nabla \times u)] = -\rho\omega^2 u$$

Bloch Theorem

- Asserts that solution in periodic potential is always a product of two terms:
  - a periodic function (with the same period)
  - a plane wave
- Mathematically, we can write:

$$\Psi(\boldsymbol{r}) = Ae^{i\boldsymbol{k}\cdot\boldsymbol{r}}u(\boldsymbol{r})$$

where $u(\boldsymbol{r}+\boldsymbol{R}) = u(\boldsymbol{r})$

Bloch Theorem

- Use Bloch's theorem to solve this eigenproblem:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\left[e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u(\boldsymbol{r})\right] = E(\boldsymbol{k})e^{i\boldsymbol{k}\cdot\boldsymbol{x}}u(\boldsymbol{r})$$

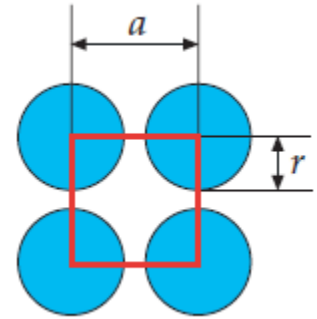
- What basis to use for periodic function?

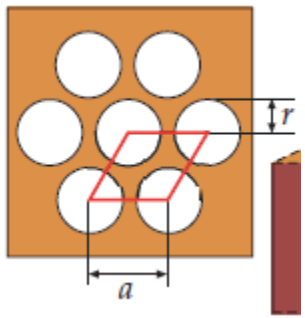
Reciprocal Lattice Vectors

- If working in Fourier space, define a set of reciprocal lattice vectors $\boldsymbol{G}$ such that $e^{i\boldsymbol{G}\cdot\boldsymbol{R}} = 1$
- Then we can construct a complex Fourier series approximating any $\boldsymbol{R}$-periodic function with: $f(\boldsymbol{r}) = \sum_{\boldsymbol{G}} f_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$
- Each coefficient calculated using orthogonality relations: $f_{\boldsymbol{G}} = \int_V d\boldsymbol{r}\, f(\boldsymbol{r}) e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}$
- In 1D lattice of period a, $\boldsymbol{G} = (2\pi m/a)\hat{x}$

Reciprocal Lattice Vectors

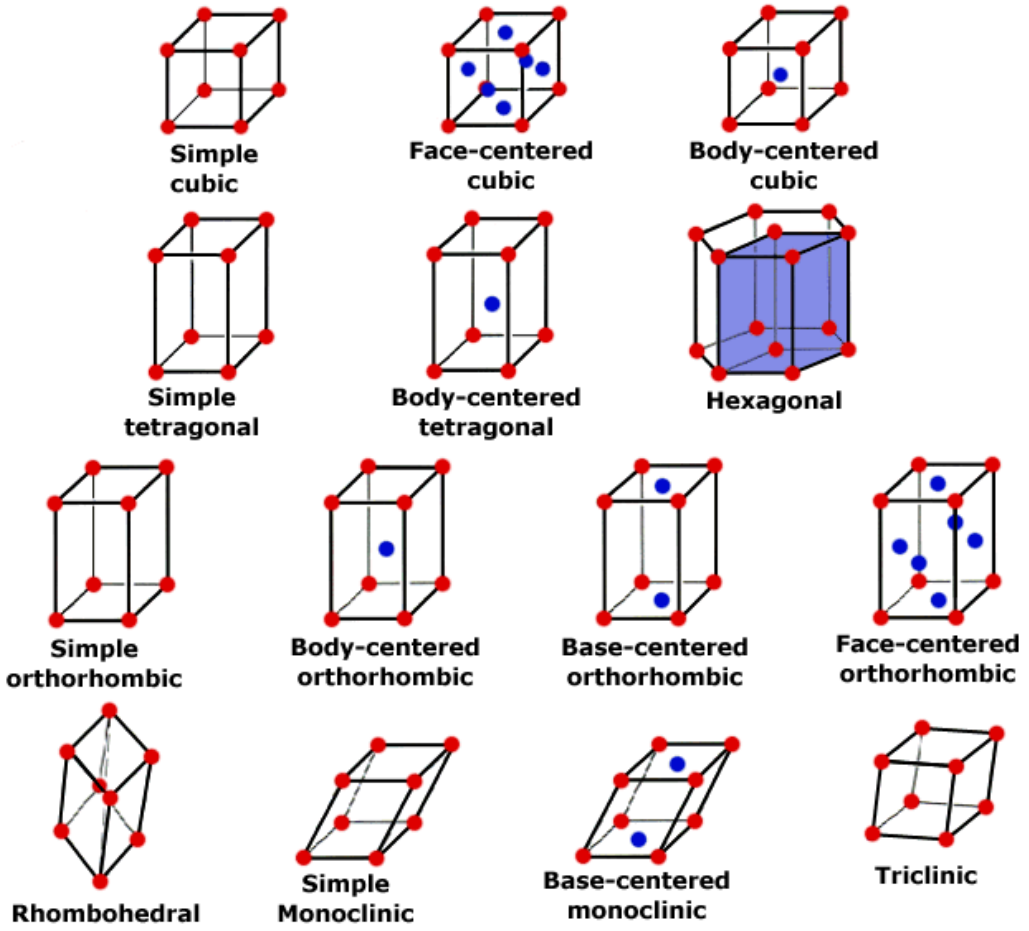
- For 2D lattice, will have two directions for our reciprocal lattice vectors, depending on lattice
- For square lattice: $G_1 = (2\pi/a)\hat{x}$; $G_2 = (2\pi/a)\hat{y}$; $\boldsymbol{G} = mG_1 + pG_2$
- For triangular lattice: $G_1 = (2\pi/a)\hat{x}$; $G_2 = (\pi/a)\left(\hat{x} + \sqrt{3}\hat{y}\right)$; $\boldsymbol{G} = mG_1 + pG_2$
- Other types include rectangular, rhombic, and oblique





Reciprocal Lattice Vectors

- In 3D, there are 14 total Bravais lattices:



Reciprocal Lattice Vectors

- In 3D, can't just construct reciprocal lattice vectors by inspection.
- If we define lattice directions $\{a_i\}$, and lattice volume $V = a_1 \cdot (a_2 \times a_3)$, then:

$$b_1 = \frac{2\pi}{V}(a_2 \times a_3)$$

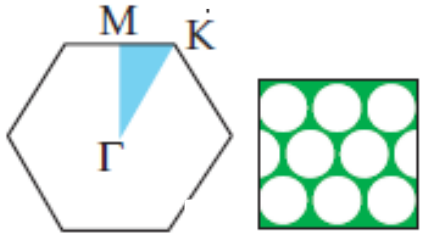
$$b_2 = \frac{2\pi}{V}(a_3 \times a_1)$$

$$b_3 = \frac{2\pi}{V}(a_1 \times a_2)$$

$$\boldsymbol{G} = mb_1 + pb_2 + qb_3$$

Reciprocal Lattice Vectors

- Brillouin Zone is constructed by drawing perpendicular bisectors between adjacent G's in reciprocal space
- BZ is where **k** can vary
- Can also introduce further symmetries to make irreducible BZ



Reciprocal Lattice Vectors

- Certain wavevectors have special designations:
  - Γ: $k = 0$ Center
  - X: $k = (\pi/a)\hat{x}$ Face center
  - L: $k = (\pi/a)(\hat{x} + \hat{y} + \hat{z})$ BZ hex face center
  - W: $k = (\pi/a)(2\hat{x} + \hat{y})$ Corner (fcc)
  - K: $k = (3\pi/2a)(\hat{x} + \hat{y})$ Edge joins hex faces
  - U: $k = (\pi/2a)(4\hat{x} + \hat{y} + \hat{z})$ Joins hex/square face
  - M: $k = (\pi/a)(\hat{x} + \hat{z})$ Center of edge

Reciprocal Lattice Vectors

- In the case of electronic bandstructures:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\Psi(x) = \hbar\omega\Psi(x)$$

- We obtain the nice recursion relation:

$$V_{G'}c_{G-G'} = \left[E(k) - \frac{\hbar^2}{2m}(k+G)^2\right]c_G$$

Reciprocal Lattice Vectors

- In the case of photonic bandstructures:

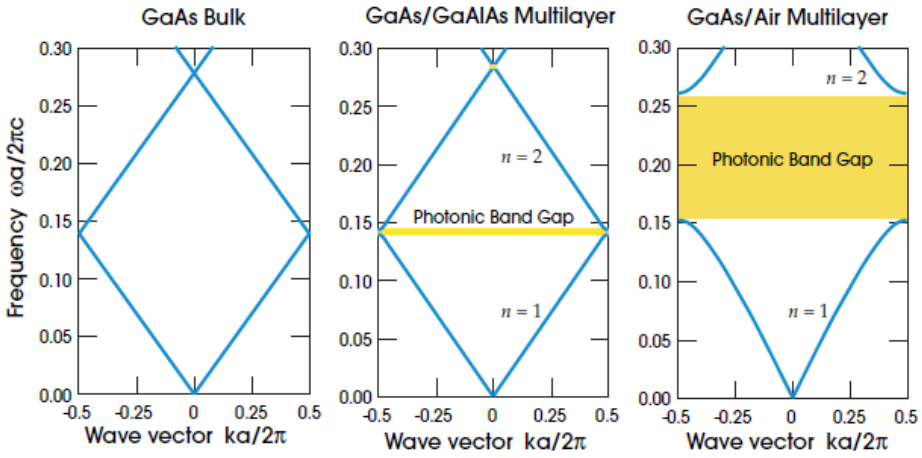
$$\nabla \times [\epsilon^{-1}(\nabla \times H)] = \left(\frac{\omega}{c}\right)^2 H$$

- We can obtain:

$$-(\boldsymbol{k}+\boldsymbol{G}) \times \left[\epsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{k}+\boldsymbol{G}') \times \boldsymbol{h}_{G-G'}\right] = \left(\frac{\omega}{c}\right)^2 \boldsymbol{h}_G$$

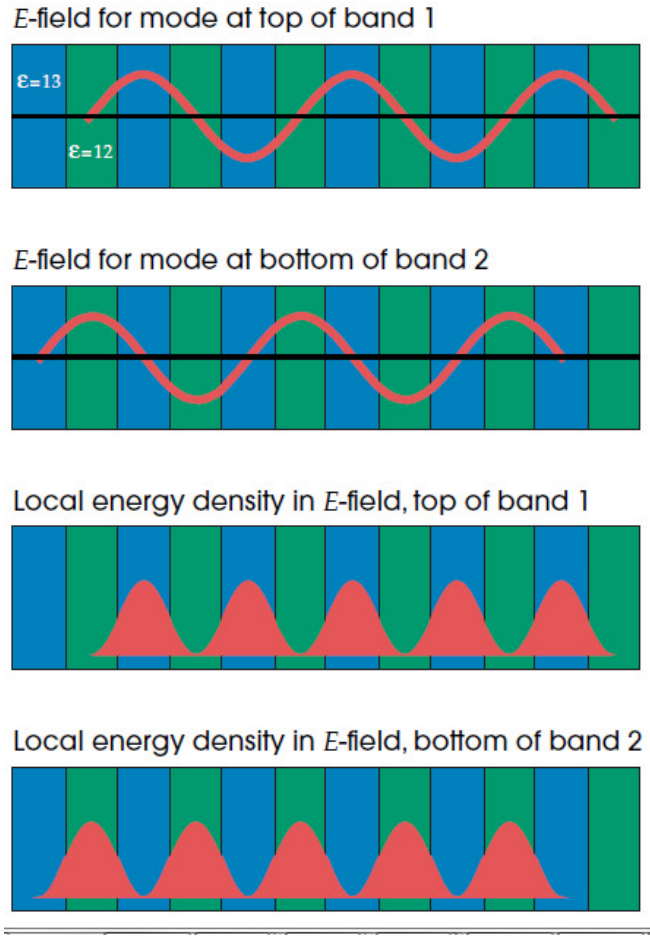
- Implemented numerically in MIT Photonic Bands (MPB): http://jdj.mit.edu/mpb/

Photonic Bandstructures: 1D

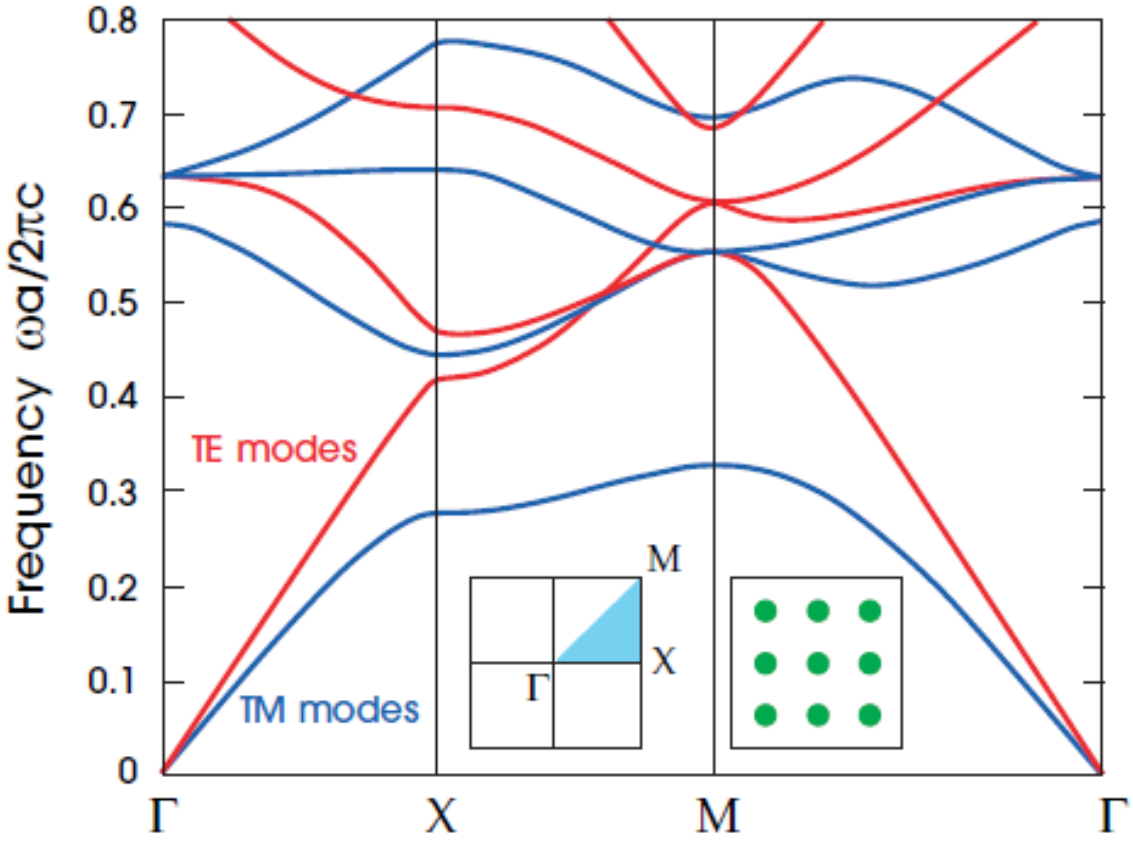


(Above) photonic bandstructures obtained for increasing dielectric contrast

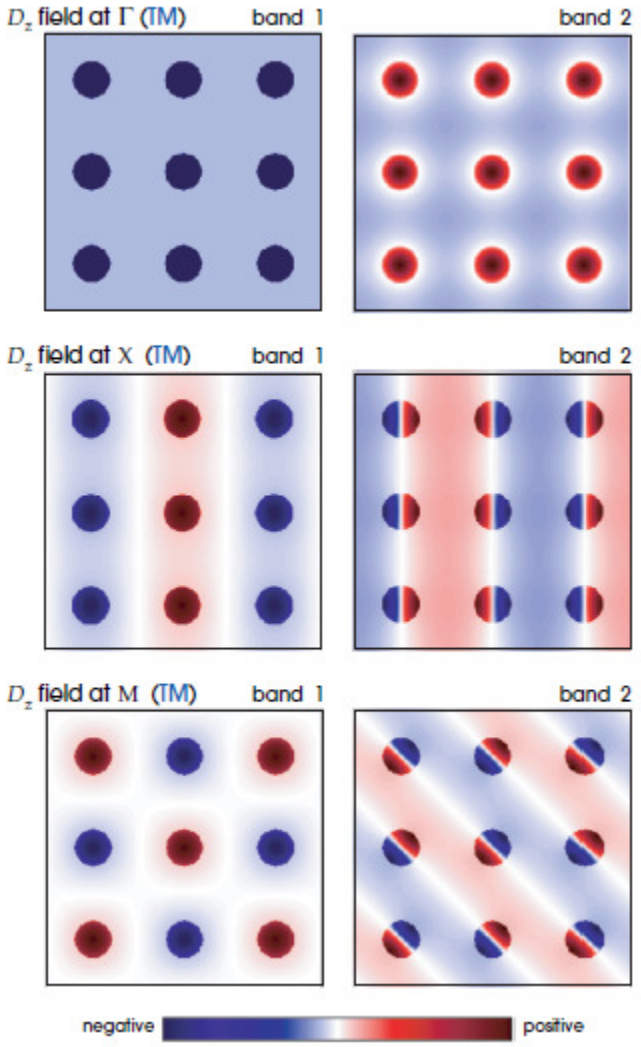
(Right) Electric fields associated with bandgap seen in middle bandstructure



Photonic Bandstructures: 2D



Photonic Bandstructures: 2D



Next Class

- Is on Wednesday, Feb. 25
- Will discuss more about bandstructures
- Recommended reading: Joannopoulos, Chapter 3 and Appendix D