Lecture #7

Theory of Periodic Structures

Lecture Outline

- Periodic devices
- Math describing periodic structures
- Electromagnetic waves in periodic structures
- Electromagnetic bands
- Isofrequency contours
- Appendix
  - Hexagonal lattices
  - Brillouin zones
Periodic Devices

Examples of Periodic Electromagnetic Devices

- Diffraction Gratings
- Waveguides
- Band Gap Materials
- Metamaterials
- Antennas
- Slow Wave Devices
- Frequency Selective Surfaces
What is a Periodic Structure?

Periodicity at the Atomic Scale

Larger-Scale Periodicity

Materials are periodic at the atomic scale. Metamaterials are periodic at a much larger scale, but smaller than a wavelength. The math describing how things are periodic is the same for both atomic scale and larger scale.

Describing Periodic Structures

• There is an infinite number of ways that structures can be periodic.
• Despite this, we need a way to describe and classify periodic lattices. We have to make generalizations to do this.
• We classify periodic structures into:
  – 230 space groups
  – 32 crystal classes
  – 14 Bravais lattices
  – 7 crystal systems

Less specific. More generalizations.
Symmetry Operations

Infinite crystals are invariant under certain symmetry operations that involve:

- Pure Translation
- Pure Rotation
- Pure Reflections
- Combinations

Definition of Symmetry Categories

- Space Groups
  - Set of all possible combinations of symmetry operations that restore the crystal to itself.
  - 230 space groups
- Bravais Lattices
  - Set of all possible ways a lattice can be periodic if composed of identical spheres placed at the lattice points.
  - 14 Bravais lattices
- Crystal Systems
  - Set of all Bravais lattices that have the same holohedry (shape of the conventional unit cell)
  - 7 crystal systems
The 14 Bravais Lattices and the Seven Crystal Systems

- Cubic
- Tetragonal
- Orthorhombic
- Monoclinic
- Triclinic
- Trigonal
- Hexagonal

Two-Dimensional Bravais Lattices

- Hexagonal: $|t_1| = |t_2|$, $\theta = 120^\circ$
- Square: $|t_1| = |t_2|$, $\theta = 90^\circ$
- Rectangular: $|t_1| \neq |t_2|$, $\theta = 90^\circ$
- Rhombic (Centered Rectangular): $|t_1| = 2 \cos \theta |t_2|$, $\theta \neq 90^\circ$
- Oblique: $|t_1| \neq |t_2|$, $\theta \neq 90^\circ$

Axis vectors = translation vectors for 2D lattices
Hybrid Symmetries

FCC Symmetry  \[ \text{Diamond = FCC + FCC} \]

Zinc Blend

Hexagonal Symmetry Has Optimal Packing Density in 2D

Electromagnetic behavior from hexagonal arrays tends to be at lower frequencies than compared to square arrays. This means feature sizes can be larger than they would be for square arrays. This is important at high frequencies and photonics where small features may be more difficult to realize.

- Square
  \[ f_{\text{sq}} = \pi \left( \frac{r}{a} \right)^2 \]
  \[ f_{\text{sq}} / \sqrt{3} = 1.1547 \]

- Hexagonal
  \[ f_{\text{hex}} = \frac{2\pi}{\sqrt{3}} \left( \frac{r}{a} \right)^2 \]
Math Describing Periodic Structures

Primitive Lattice Vectors

Axis vectors most intuitively define the shape and orientation of the unit cell. They cannot uniquely describe all 14 Bravais lattices, but they do uniquely identify the 7 crystal systems.

Translation vectors connect adjacent points in the lattice and can uniquely describe all 14 Bravais lattices. They are less intuitive to interpret.

Primitive lattice vectors are the smallest possible vectors that still describe the unit cell.
## Axis → Translation Vectors

**Simple**
\[
\begin{bmatrix}
\hat{t}_x \\
\hat{t}_y \\
\hat{t}_z
\end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \end{bmatrix} \begin{bmatrix}
\hat{a}_x \\
\hat{a}_y \\
\hat{a}_z
\end{bmatrix}
\]

**Body-Centered**
\[
\begin{bmatrix}
\hat{t}_x \\
\hat{t}_y \\
\hat{t}_z
\end{bmatrix} = \begin{bmatrix} -1/2 & 1/2 & 1/2 \\
1/2 & 1/2 & 1/2 \\
1/2 & 1/2 & -1/2 \end{bmatrix} \begin{bmatrix}
\hat{a}_x \\
\hat{a}_y \\
\hat{a}_z
\end{bmatrix}
\]

**Face-Centered**
\[
\begin{bmatrix}
\hat{t}_x \\
\hat{t}_y \\
\hat{t}_z
\end{bmatrix} = \begin{bmatrix} 0 & 1/2 & 1/2 \\
1/2 & 0 & 1/2 \\
1/2 & 1/2 & 0 \end{bmatrix} \begin{bmatrix}
\hat{a}_x \\
\hat{a}_y \\
\hat{a}_z
\end{bmatrix}
\]

**Base-Centered**
\[
\begin{bmatrix}
\hat{t}_x \\
\hat{t}_y \\
\hat{t}_z
\end{bmatrix} = \begin{bmatrix} -1/2 & 1/2 & 0 \\
1/2 & 1/2 & 0 \\
0 & 0 & 1/2 \end{bmatrix} \begin{bmatrix}
\hat{a}_x \\
\hat{a}_y \\
\hat{a}_z
\end{bmatrix}
\]

**Trigonal**
\[
\begin{bmatrix}
\hat{t}_x \\
\hat{t}_y \\
\hat{t}_z
\end{bmatrix} = \begin{bmatrix} 1 & 1/3 & 1/3 \\
-1/3 & 1/3 & 1/3 \\
-1/3 & -1 & 1/3 \end{bmatrix} \begin{bmatrix}
\hat{a}_x \\
\hat{a}_y \\
\hat{a}_z
\end{bmatrix}
\]

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## Non-Primitive Lattice Vectors

Almost always, the label “lattice vector” refers to the translation vectors, not the axis vectors.

A translation vector is any vector that connects two points in a lattice. They must be an integer combination of the primitive translation vectors.

\[
\vec{t}_{pqr} = pt_1 + qt_2 + rt_3 \\
p = \cdots, -2, -1, 0, 1, 2, \cdots \\
q = \cdots, -2, -1, 0, 1, 2, \cdots \\
r = \cdots, -2, -1, 0, 1, 2, \cdots
\]
Reciprocal Lattices (1 of 2)

Each direct lattice has a unique reciprocal lattice so knowledge of one implies knowledge of the other.

Reciprocal Lattices (2 of 2)

<table>
<thead>
<tr>
<th>Direct Lattice</th>
<th>Reciprocal Lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple Cubic</td>
<td>Simple Cubic</td>
</tr>
<tr>
<td>Body-Centered Cubic</td>
<td>Face-Centered Cubic</td>
</tr>
<tr>
<td>Face-Centered Cubic</td>
<td>Body-Centered Cubic</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>Hexagonal</td>
</tr>
</tbody>
</table>
Reciprocal Lattice Vectors for 3D Lattices

The reciprocal lattice vectors can be calculated from the direct lattice vectors (and the other way around) as follows:

\[ \vec{\mathbf{T}}_1 = 2\pi \frac{\vec{\mathbf{t}}_2 \times \vec{\mathbf{t}}_3}{\vec{\mathbf{t}}_1 \cdot (\vec{\mathbf{t}}_2 \times \vec{\mathbf{t}}_3)} \quad \vec{\mathbf{T}}_2 = 2\pi \frac{\vec{\mathbf{t}}_3 \times \vec{\mathbf{t}}_1}{\vec{\mathbf{t}}_2 \cdot (\vec{\mathbf{t}}_3 \times \vec{\mathbf{t}}_1)} \quad \vec{\mathbf{T}}_3 = 2\pi \frac{\vec{\mathbf{t}}_1 \times \vec{\mathbf{t}}_2}{\vec{\mathbf{t}}_3 \cdot (\vec{\mathbf{t}}_1 \times \vec{\mathbf{t}}_2)} \]

There also exists primitive reciprocal lattice vectors. All reciprocal lattice vectors must be an integer combination of the primitive reciprocal lattice vectors.

\[ \vec{\mathbf{T}}_{PQR} = P \vec{\mathbf{T}}_1 + Q \vec{\mathbf{T}}_2 + R \vec{\mathbf{T}}_3 \]

\[ P = \cdots, -2, -1, 0, 1, 2, \cdots \]
\[ Q = \cdots, -2, -1, 0, 1, 2, \cdots \]
\[ R = \cdots, -2, -1, 0, 1, 2, \cdots \]

Reciprocal Lattice Vectors for 2D Lattices

The reciprocal lattice vectors can be calculated from the direct lattice vectors (and the other way around) as follows:

\[ \vec{\mathbf{T}}_1 = \frac{2\pi}{\vec{\mathbf{t}}_1 \cdot \vec{\mathbf{t}}_2} \begin{bmatrix} t_{2,y} \\ -t_{2,x} \end{bmatrix} \quad \vec{\mathbf{T}}_2 = \frac{2\pi}{\vec{\mathbf{t}}_1 \cdot \vec{\mathbf{t}}_2} \begin{bmatrix} -t_{1,y} \\ t_{1,x} \end{bmatrix} \]

\[ \vec{\mathbf{t}}_1 = \frac{2\pi}{\vec{\mathbf{t}}_1 \cdot \vec{\mathbf{t}}_2} \begin{bmatrix} T_{2,y} \\ -T_{2,x} \end{bmatrix} \quad \vec{\mathbf{t}}_2 = \frac{2\pi}{\vec{\mathbf{t}}_1 \cdot \vec{\mathbf{t}}_2} \begin{bmatrix} -T_{1,y} \\ T_{1,x} \end{bmatrix} \]
Grating Vector, $\vec{K}$

A grating vector is very much like a wave vector in that its direction is normal to planes and its magnitude is $2\pi$ divided by the spacing between the planes.

\[ |\vec{K}| = \frac{2\pi}{\Lambda} \]

\[ \vec{K} = K_x \hat{x} + K_y \hat{y} + K_z \hat{z} \]

Reciprocal Lattice Vectors are Grating Vectors

Reciprocal lattice vectors are grating vectors!!

\[ \vec{T}_a \rightarrow \vec{K}_a = \frac{2\pi}{\Lambda_a} \]

There is a close and elegant relationship between the reciprocal lattice vectors and wave vectors. For this reason, periodic structures are often analyzed in reciprocal (grating vector) space.
Miller Indices

Miller indices identify repeating planes within periodic structures like crystals.

Recall the definition of a reciprocal lattice vector...

\[ \vec{T}_{PQR} = P\vec{T}_1 + Q\vec{T}_2 + R\vec{T}_3 \]

\(P, Q,\) and \(R\) are the Miller indices of the planes described by the reciprocal lattice vector \(\vec{T}_{PQR}\).

\[ \langle PQR \rangle \]

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### Primitive Unit Cells

Primitive unit cells are the smallest volume of space that can be stacked onto itself (with no voids and no overlaps) to correctly reproduce the entire lattice.

The Wigner-Seitz cell is one method of constructing a primitive unit cell. It is defined as the volume of space around a single point in the lattice that is closer to that point than any other point in the lattice. A proper unit cell contains only one “atom.”

These illustrations show the relationship between the conventional unit cell (shown as frames) and the Wigner-Seitz cell (shown as volumes) for the three cubic lattices.
Constructing the Wigner-Seitz Primitive Unit Cell (1 of 2)

BCC Conventional Unit Cell

Wigner-Seitz Unit Cell

How to we construct this?

Constructing the Wigner-Seitz Primitive Unit Cell (2 of 2)

Step 1 – Pick a point in the lattice to build the unit cell around.
Step 2 – Construct planes that bisect the region between all adjacent points.
Step 3 – The unit cell is the region enclosed by all of the planes.
The Brillouin zone is constructed in the same manner as the Wigner-Seitz unit cell, but it is constructed from the reciprocal lattice.

The Brillouin zone is closely related to wave vectors and diffraction so analysis of periodic structures is often performed in “reciprocal space.”

The Brillouin zone for a face-centered-cubic lattice is a “truncated” octahedron with 14 sides.

This is the most “spherical” of all the Brillouin zones so the FCC lattice is said to have the highest symmetry of the Bravais lattices.

Of the FCC lattices, diamond has the highest symmetry.

Different Brillouin Zones

http://www.eelvex.net/physics/finding-brillouin-zones-a-visual-guide/
Degree of Symmetry

The *degree of symmetry* refers to how spherical the Brillouin zone is.

<table>
<thead>
<tr>
<th>Lowest Symmetry</th>
<th>Highest Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triclinic</td>
<td>Pseudo-periodic</td>
</tr>
<tr>
<td>SC</td>
<td>Diamond (FCC)</td>
</tr>
<tr>
<td>BCC</td>
<td></td>
</tr>
<tr>
<td>FCC</td>
<td></td>
</tr>
</tbody>
</table>

Exploiting Additional Symmetry

If the field is known at every point inside a single unit cell, then it is also known at any point in an infinite lattice because the field takes on the same symmetry as the lattice so it just repeats itself.

Since the reciprocal lattice uniquely defines a direct lattice, knowing the solutions to the wave equation at each point inside the reciprocal lattice unit cell also defines the solution everywhere in the infinite reciprocal lattice.

Many times, there is still additional symmetry to exploit. So, the smallest volume of space that completely describes the electromagnetic wave can be smaller than the unit cell itself.

Due to the symmetry in this example, the field at any point in the entire lattice can be mapped to an equivalent point in this triangle.

The field in each of these squares is a mirror image of each other.
The Irreducible Brillouin Zone

The smallest volume of space within the Brillouin zone that completely characterizes the periodic structure is called the irreducible Brillouin zone (IBZ). It is smaller than the Brillouin zone when there is additional symmetry to exploit.

Electromagnetic Waves in Periodic Structures
Waves are Perturbed by Objects

When a portion of a wave propagates through an object, that portion is delayed.

Thus, a wave gets perturbed by the object.

Fields in Periodic Structures

Waves in periodic structures take on the same symmetry and periodicity as their host.
The Bloch Theorem

Waves inside of a periodic structure are like plane waves, but they are modulated by an envelope function. It is the envelope function that takes on the same symmetry and periodicity as the structure.

\[ \vec{E}(\vec{r}) = \vec{A}(\vec{r}) e^{i\vec{\beta} \cdot \vec{r}} \]

Overall field is the combination of the envelope and plane wave term.

Envelope function has the same symmetry and periodicity as the periodic structure.

Plane-wave like phase “tilt” term.

\( \vec{\beta} = \text{Bloch wave vector} \)

Example Waves in a Periodic Lattice

Wave normally incident onto a periodic structure.

Wave incident at 45° onto the same periodic structure.
Mathematical Description of Periodicity

A structure is periodic if its material properties repeat. Given the lattice vectors, the periodicity is expressed as

\[ \varepsilon (\vec{r} + \vec{t}_{pqr}) = \varepsilon (\vec{r}) \quad \vec{t}_{pqr} = p\vec{t}_1 + q\vec{t}_2 + r\vec{t}_3 \]

Recall that it is the amplitude of the Bloch wave that has the same periodicity as the structure the wave is in. Therefore,

\[ A(\vec{r} + \vec{t}_{pqr}) = A(\vec{r}) \quad \vec{t}_{pqr} = p\vec{t}_1 + q\vec{t}_2 + r\vec{t}_3 \]

Example – 1D Periodicity

Many devices are periodic along just one dimension.

For a device that is periodic only along one direction, these relations reduce to

\[ \varepsilon (x + p\Lambda_x, y, z) = \varepsilon (x, y, z) \quad \varepsilon (x + p\Lambda_x) = \varepsilon (x) \]
\[ A(x + p\Lambda_x, y, z) = A(x, y, z) \quad A(x + p\Lambda_x) = A(x) \]

\( p = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty \)
Electromagnetic Bands

Band Diagrams (1 of 2)

Band diagrams are a compact, but incomplete, means of characterizing the electromagnetic properties of a periodic structure. It is essentially a map of the frequencies of the eigen-modes as a function of the Bloch wave vector $\beta$.

\[ |\beta| = \frac{2\pi}{\lambda} \]

$\beta$ is Bloch wave vector.

\[ \nabla \times \frac{1}{\varepsilon_r} \nabla \times \vec{H} = k_{0,\beta}^2 \vec{H} \]

$\vec{H}_{i,\beta}$ is Eigen-Vector, $i = 1, \infty$.
Band Diagrams (2 of 2)

To construct a band diagram, we make small steps around the perimeter of the irreducible Brillouin zone (IBZ) and compute the eigen-values at each step. When we plot all these eigen-values as a function of \( \beta \), the points line up to form continuous “bands.”

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Animation of the Construction of a Band Diagram

FCC Brillouin Zone

Photonic Band Diagram

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At least five electromagnetic properties can be estimated from a band diagram.

- **Band gaps**
  - Absence of any bands within a range of frequencies indicates a band gap.
  - A COMPLETE BAND GAP is one that exists over all possible Bloch wave vectors.

- **Transmission/reflection spectra**
  - Band gaps lead to suppressed transmission and enhanced reflection

- **Phase velocity**
  - The slope of the line connecting $\Gamma$ to the point on the band corresponds to phase velocity.
  - From this, we get the effective phase refractive index.

- **Group velocity**
  - The slope of the band at the point of interest corresponds to the group velocity.
  - From this, we get the effective group refractive index.

- **Dispersion**
  - Any time the band deviates from the “light line” there is dispersion.
  - The phase and group velocity are the same except when there is dispersion.
The Band Diagram is Missing Information

Direct lattice: We have an array of air holes in a dielectric with $n=3.0$.

Reciprocal lattice: We construct the band diagram by marching around the perimeter of the irreducible Brillouin zone.

The band extremes "almost" always occur at the key points of symmetry.

But we are missing information from inside the Brillouin zone.
The Complete Band Diagram

The Full Brillouin Zone...

There is an infinite set of eigen-frequencies associated with each point in the Brillouin zone. These form "sheets" as shown at right.

Animation of Complete Photonic Band Diagram

Lecture 7
Relation Between the Complete Band Diagram and the Band Diagram (1 of 4)

We start with the full band diagram.

Relation Between the Complete Band Diagram and the Band Diagram (2 of 4)

We raise walls around the perimeter of the irreducible Brillouin zone.

These walls slice through the bands.
We focus only on the intersections of the walls and the bands.

We unfold the walls to reveal the ordinary band diagram.
Calculating Isofrequency Contours (i.e. Index Ellipsoids for Periodic Structures)

Recall Phase Vs. Power Flow

*Isotropic Materials*

Phase propagates in the direction of \( \mathbf{k} \). Therefore, the refractive index derived from \(|\mathbf{k}|\) is best described as the phase refractive index. Velocity here is the phase velocity.

*Anisotropic Materials*

Energy propagates in the direction of \( \mathbf{P} \) which is always normal to the surface of the index ellipsoid. From this, we can define a group velocity and a group refractive index.
Isofrequency contours are mostly circular. Not much interesting here.

Isofrequency From Second-Order Band

Index ellipsoids are “isofrequency contours” in k-space.
Index ellipsoids in periodic structures are very interesting and useful because they can be things other than ellipsoids. They tend to resemble the shape of the Brillouin zone.

Example Applications

Self-Collimation

Negative Refraction
Geometry of a Hexagonal Lattice (2 of 3)

Direct Lattice

Reciprocal Lattice

\[ \vec{t}_1 = \frac{a}{2} \hat{x} - \frac{a\sqrt{3}}{2} \hat{y} \]
\[ \vec{t}_2 = \frac{a}{2} \hat{x} + \frac{a\sqrt{3}}{2} \hat{y} \]
\[ \vec{t}_3 = c \hat{z} \]

\[ \vec{t}_1' = \frac{2\pi}{a} \hat{x} - \frac{2\pi}{a\sqrt{3}} \hat{y} \]
\[ \vec{t}_2' = \frac{2\pi}{a} \hat{x} + \frac{2\pi}{a\sqrt{3}} \hat{y} \]
\[ \vec{t}_3' = \left(\frac{2\pi}{c}\right) \hat{z} \]

Geometry of a Hexagonal Lattice (3 of 3)

Brillouin Zone and Irreducible Brillouin Zone

\( \Gamma = 0 \)
\( \mathbf{M} = \frac{1}{2} \vec{T}_2 \)
\( \mathbf{K} = \frac{1}{3} \vec{T}_1 + \frac{1}{3} \vec{T}_2 \)
\( \mathbf{A} = \frac{1}{2} \vec{T}_3 \)
\( \mathbf{L} = \frac{1}{2} \vec{T}_2 + \frac{1}{2} \vec{T}_3 \)
\( \mathbf{H} = \frac{1}{3} \vec{T}_1 + \frac{1}{3} \vec{T}_2 + \frac{1}{2} \vec{T}_3 \)