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Advanced Electromagnetics:
21st Century Electromagnetics

Unit Cells & Brillouin Zones

Lecture Outline

- Physical interpretation of reciprocal lattice vectors
- Unit cells & the Brillouin zone
- The irreducible Brillouin zone (IBZ)
- Degree of symmetry

Physical Interpretation of Reciprocal Lattice Vectors

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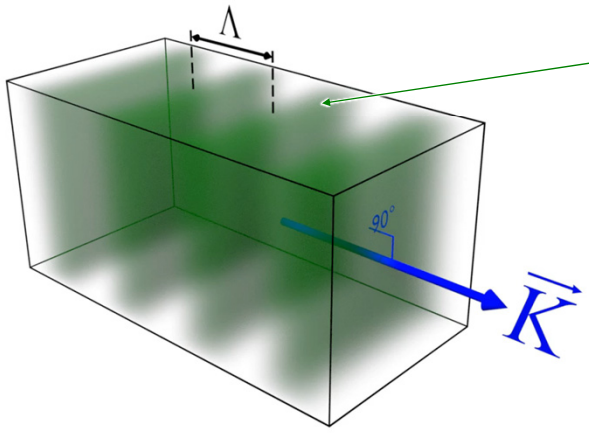
Grating Vector $\vec{K}$

A grating vector $\vec{K}$ is very much like a wave vector $\vec{k}$ in that its direction is normal to repeating planes and its magnitude is 2π divided by the spacing between the planes.



$$\varepsilon_r(\vec{r}) = \varepsilon_{avg} + \Delta\varepsilon \cos\left(\vec{K} \bullet \vec{r}\right)$$

$$\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$$

position vector

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

$$\left|\vec{K}\right| = \frac{2\pi}{\Lambda}$$

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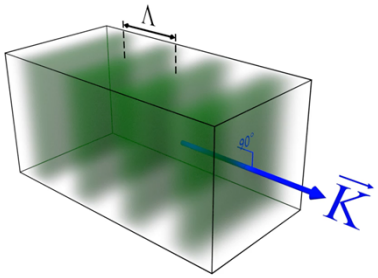
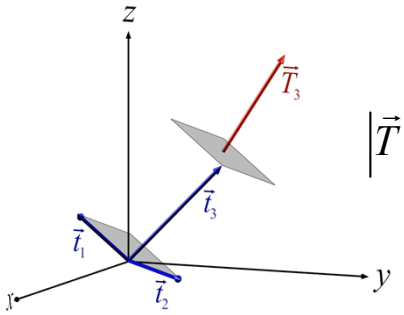
Reciprocal Lattice Vectors & Grating Vectors



$$\left|\vec{K}\right| = \frac{2\pi}{\Lambda}$$



$$\left|\vec{T}\right| = \frac{2\pi}{\Lambda}$$

Reciprocal lattice vectors are grating vectors!!

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 space.

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Miller Indices

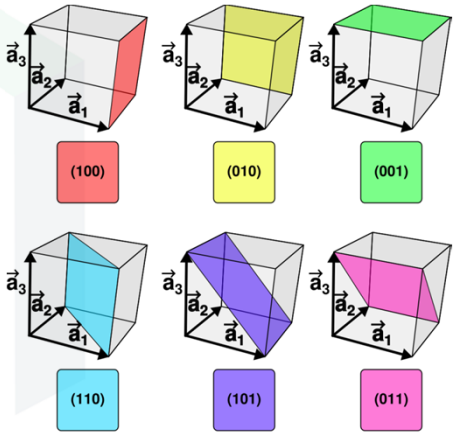
Miller indices identify repeating planes within periodic structures like crystals.

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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Unit Cells & the Brillouin Zone

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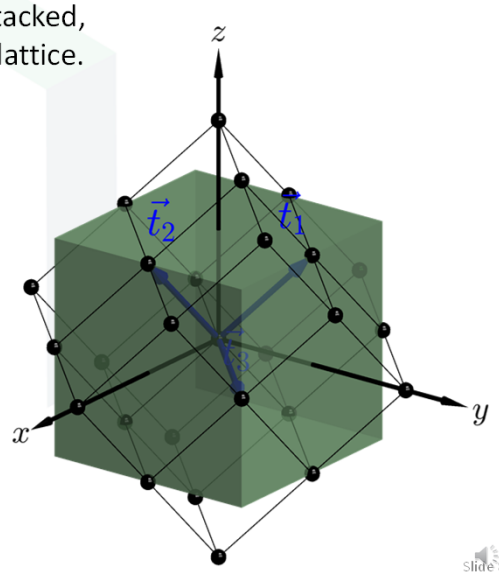
Conventional Unit Cell

A *unit cell* is a piece of a periodic structure that when stacked, without any overlaps or voids, perfectly constructs the lattice.

The *conventional unit cell* illustrates the periodic structure most intuitively, but it is not the only choice for a unit cell and is usually not the smallest.

For numerical analysis, the smallest possible volume is desired because this minimizes the volume of space that is analyzed



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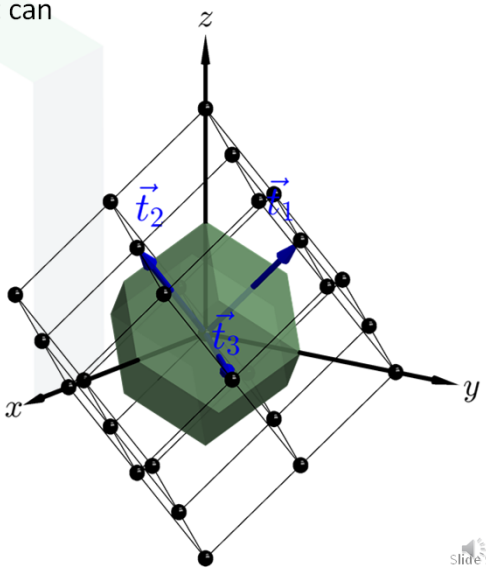
Wigner-Seitz Primitive Unit Cell

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 primitive unit cell contains only one "atom."



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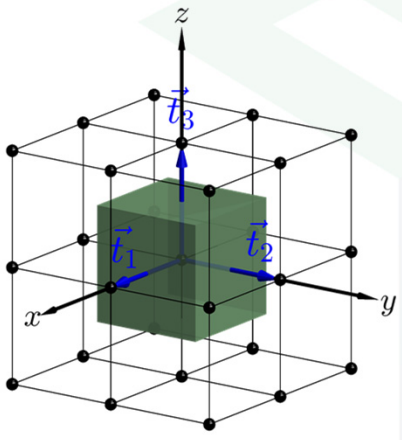
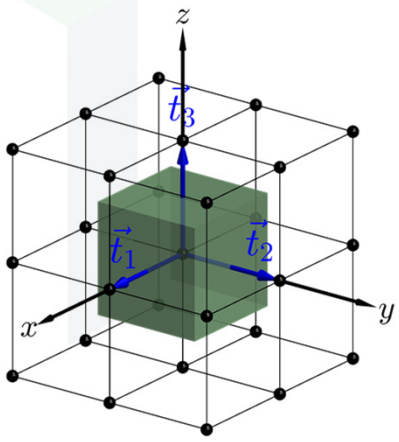
Conventional Vs. Wigner-Seitz Unit Cells for Simple Cubic

Conventional



Wigner-Seitz



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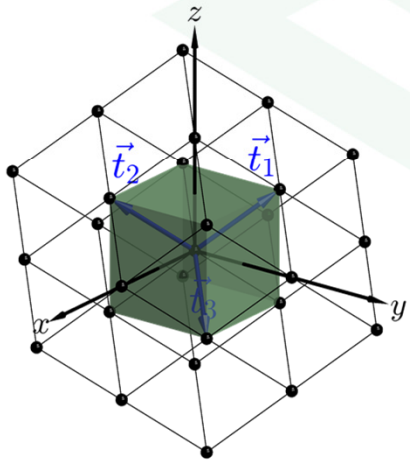
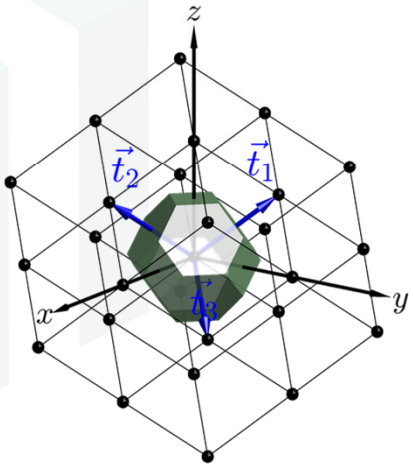
Conventional Vs. Wigner-Seitz Unit Cells for Body-Centered Cubic

Conventional



Wigner-Seitz



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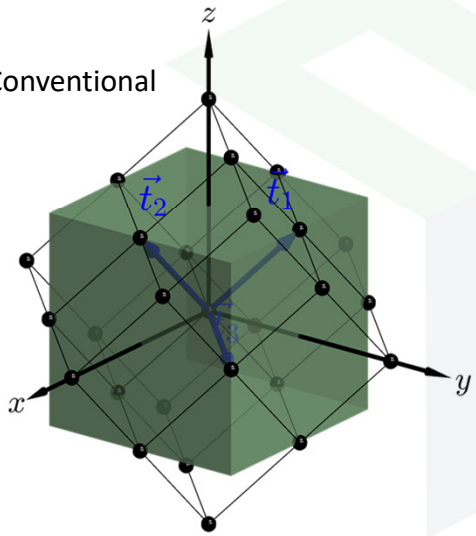
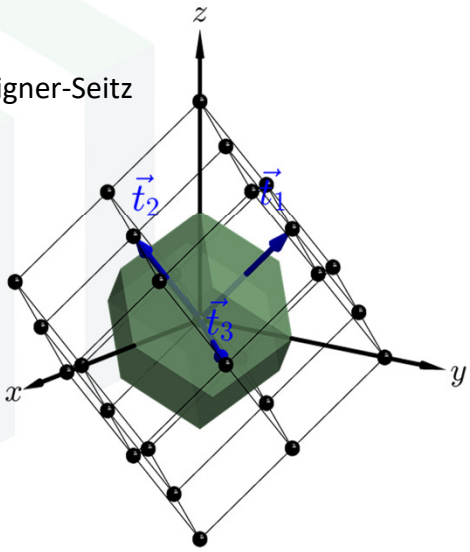
Conventional Vs. Wigner-Seitz Unit Cells for Face-Centered Cubic

Conventional



Wigner-Seitz



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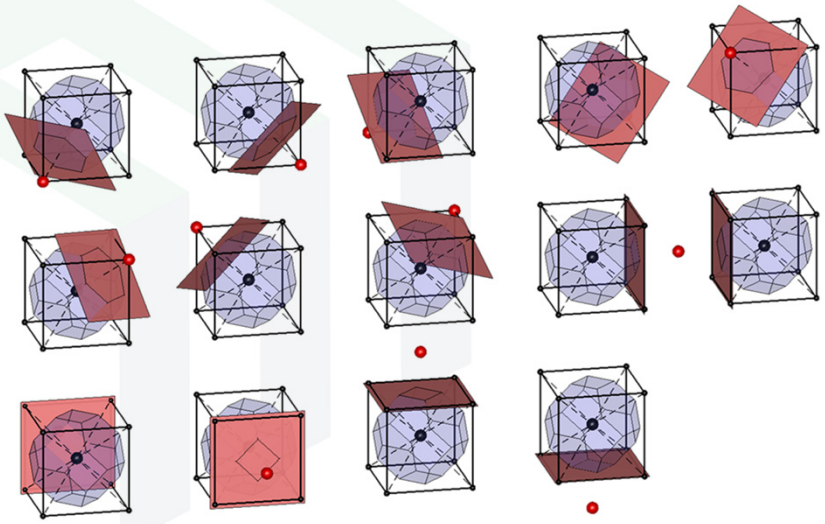
Constructing the Wigner-Seitz Primitive Unit Cell

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.

* Algorithm is the same as Voronoi tessellation.



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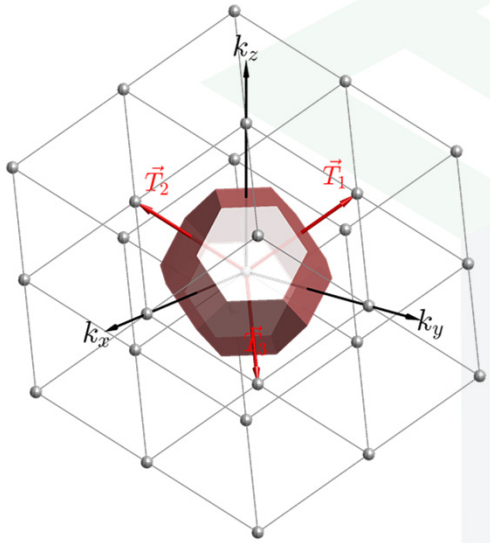
The Brillouin Zone



The *Brillouin zone* is the Wigner-Seitz unit cell constructed from the reciprocal lattice.

It is essentially a map of the periodicity of the lattice as a function of direction.

Shown here is the Brillouin zone for a face-centered cubic lattice. It is a truncated octahedron and has 14 sides.

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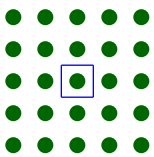
The Irreducible Brillouin Zone (IBZ)

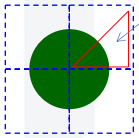
Exploiting Additional Symmetry

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 Brillouin zone 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.





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

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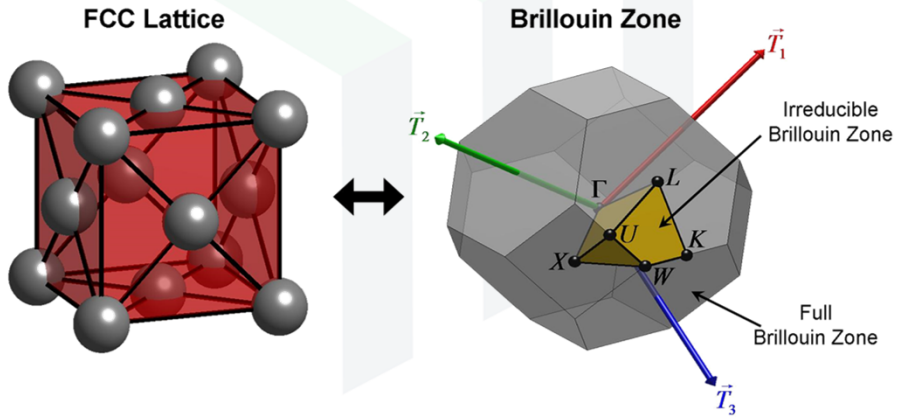
The Irreducible Brillouin Zone (IBZ)

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.



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Degree of Symmetry

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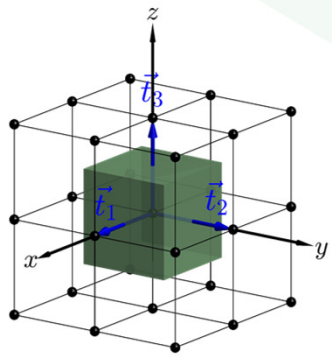
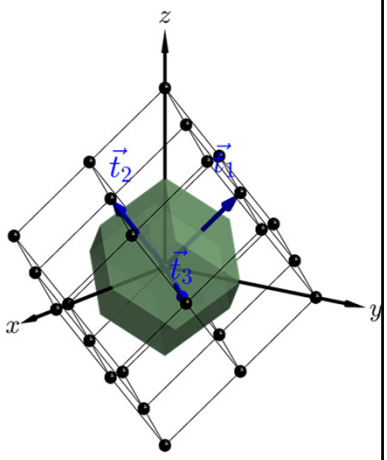
Which Lattice Has the Most Spherical Wigner-Seitz Unit Cell?

Simple Cubic



Body-Centered Cubic

Face-Centered Cubic



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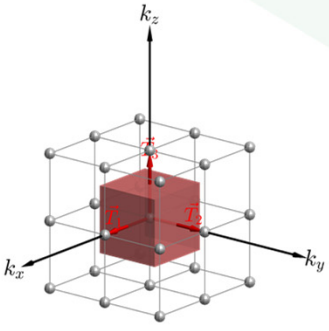
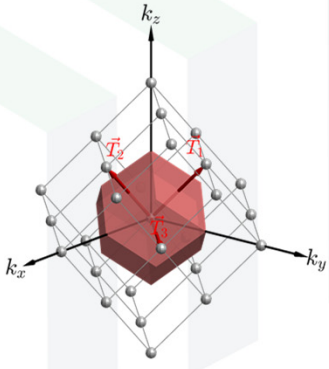
Which Lattice Has the Most Spherical Brillouin Zone?

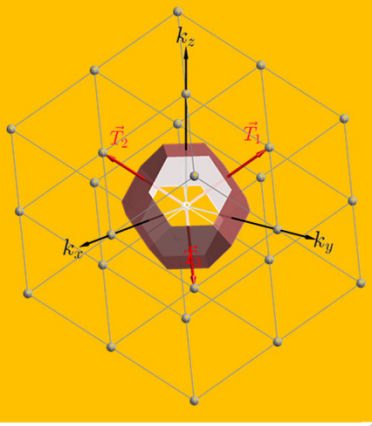
Simple Cubic



Body-Centered Cubic



Face-Centered Cubic



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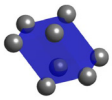
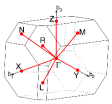
Degree of Symmetry

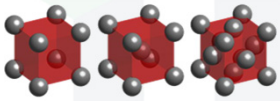
The *degree of symmetry* refers to how spherical the Brillouin zone is.

Lowest Symmetry → Highest Symmetry



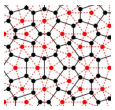
Triclinic





SC BCC FCC

Diamond (FCC)



Pseudo-periodic

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