Section 8
Brillouin Zone and Reciprocal Lattice

8.3 3D Problems

Gerhard Klimeck
gekco@purdue.edu

PURDUE UNIVERSITY

School of Electrical and Computer Engineering

Section 8
Brillouin Zone and Reciprocal Lattice

One Video Segment

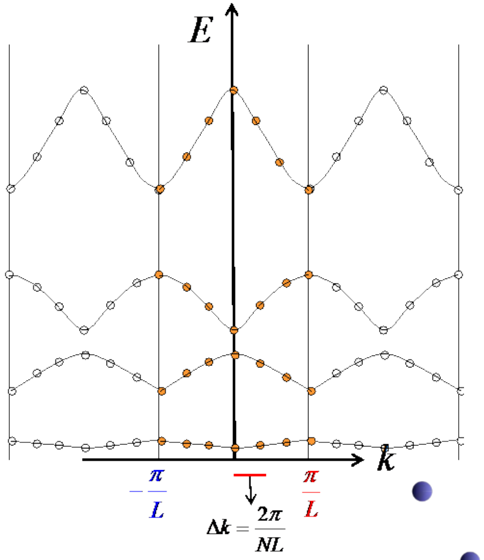
- 8.1 1D Problems
  - » Brillouin Zone
  - » Solution strategy
  - » Reciprocal Lattice

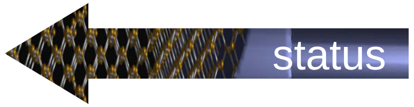
One Video Segment

- 8.2 2D Problems
  - » Reciprocal Lattice Recipe
  - » Examples - Square and Hexagonal

One Video Segment

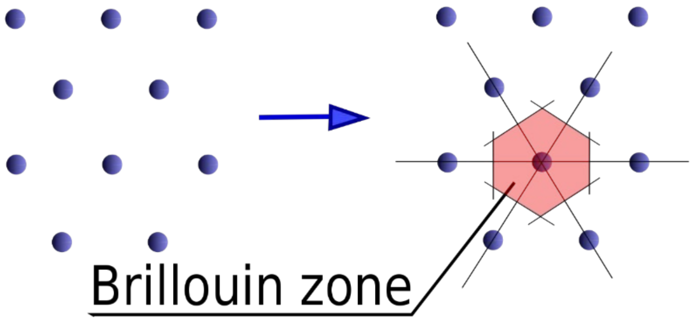
- 8.3 3D Problems
  - » Reciprocal Lattice Recipe
  - » Examples





$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$$

$$\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$$



$$\boldsymbol{b}_1 = 2\pi \frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot \bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2}$$

$$\boldsymbol{b}_2 = 2\pi \frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1}{\boldsymbol{a}_2 \cdot \bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1}$$

$$\cos\theta = \boldsymbol{a}_1 \cdot \boldsymbol{a}_2$$

$$\bar{\bar{\boldsymbol{R}}} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

Prasad Sarangapani, Arun Goud Akkala, Sebastian Steiger, Hong-Hyun Park, Yosef Borga, Tillmann Christoph Kubis, Michael Povolotskyi, Gerhard Klimeck (2014), "Brillouin Zone Viewer," https://nanohub.org/resources/brillouin. (DOI: 10.4231/D3DB7VQ35).

Reciprocal Spaces of 2D & 3D Bravais Lattices

$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$ $\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$ $\boldsymbol{a}_1, \boldsymbol{a}_2$ Primitive Bravais Lattice Vectors

n_1, n_2, m_1, m_2 Any integer

$$\sum_m f_m e^{i\mathbf{G}_m\cdot\mathbf{r}} = f(\mathbf{r})$$ $\boldsymbol{G}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$ => Reciprocal Space Basis

$$\boldsymbol{b}_1 = 2\pi\frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2}{\boldsymbol{a}_1\cdot\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2} \quad \boldsymbol{b}_2 = 2\pi\frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1}{\boldsymbol{a}_2\cdot\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1} \quad \bar{\bar{\boldsymbol{R}}} = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix} \quad \cos\theta = \boldsymbol{a}_1\cdot\boldsymbol{a}_2$$

$\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$ $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ Primitive Bravais Lattice Vectors

n_1, n_2, n_3 Any integer

$\boldsymbol{G}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2 + m_3\boldsymbol{b}_3$ m_1, m_2, m_3

$$\boldsymbol{b}_1 = 2\pi\frac{\boldsymbol{a}_2\times\boldsymbol{a}_3}{\boldsymbol{a}_1\cdot(\boldsymbol{a}_2\times\boldsymbol{a}_3)} \quad \boldsymbol{b}_2 = 2\pi\frac{\boldsymbol{a}_3\times\boldsymbol{a}_1}{\boldsymbol{a}_2\cdot(\boldsymbol{a}_3\times\boldsymbol{a}_1)} \quad \boldsymbol{b}_3 = 2\pi\frac{\boldsymbol{a}_1\times\boldsymbol{a}_2}{\boldsymbol{a}_3\cdot(\boldsymbol{a}_1\times\boldsymbol{a}_2)}$$

Do a quick sanity check! $\mathbf{G}_m\cdot\mathbf{R}_n = 2\pi N$

This is the full 3D Recipe!

https://en.wikipedia.org/wiki/Reciprocal_lattice

$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n) \qquad \sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$$

$$\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$$

$\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ Primitive Bravais Lattice Vectors

n_1, n_2, n_3 Any integer

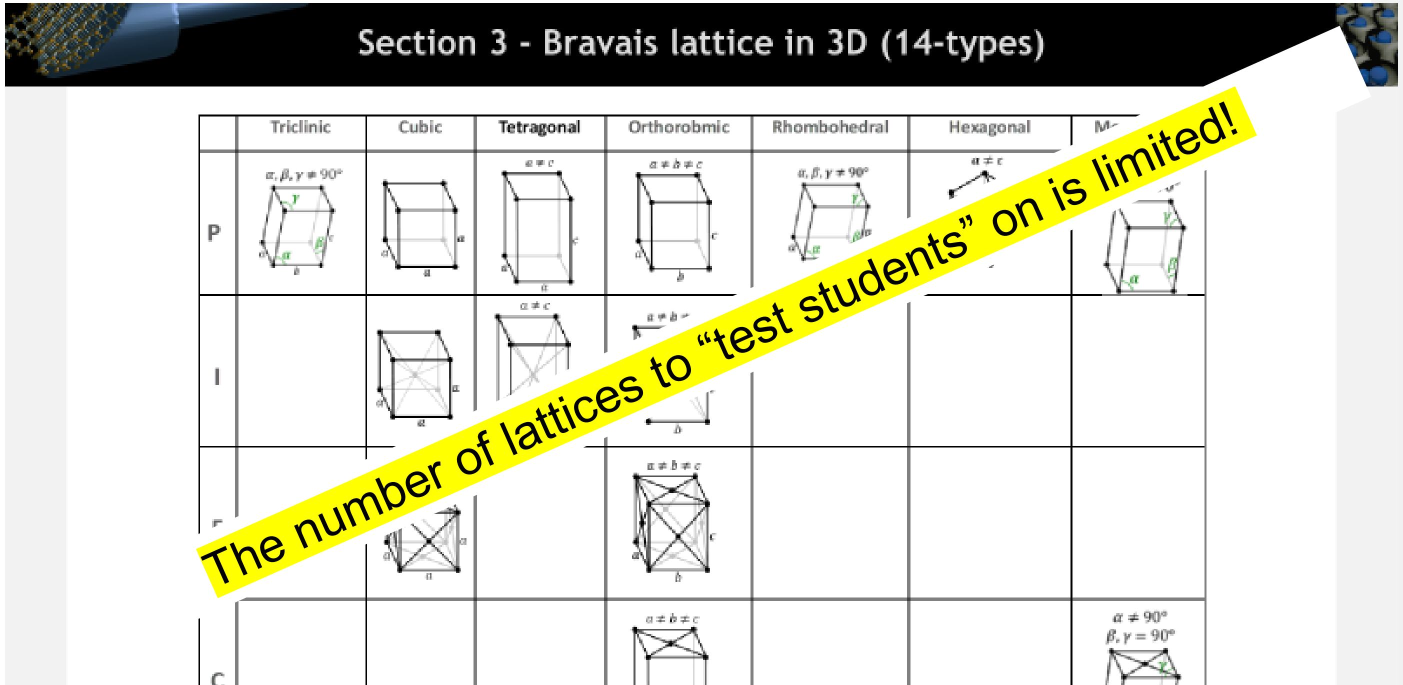
m_1, m_2, m_3

$$\boldsymbol{G}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2 + m_3\boldsymbol{b}_3$$

$$\boldsymbol{b}_1 = 2\pi\frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} \qquad \boldsymbol{b}_2 = 2\pi\frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_2 \cdot (\boldsymbol{a}_3 \times \boldsymbol{a}_1)} \qquad \boldsymbol{b}_3 = 2\pi\frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\boldsymbol{a}_3 \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2)}$$

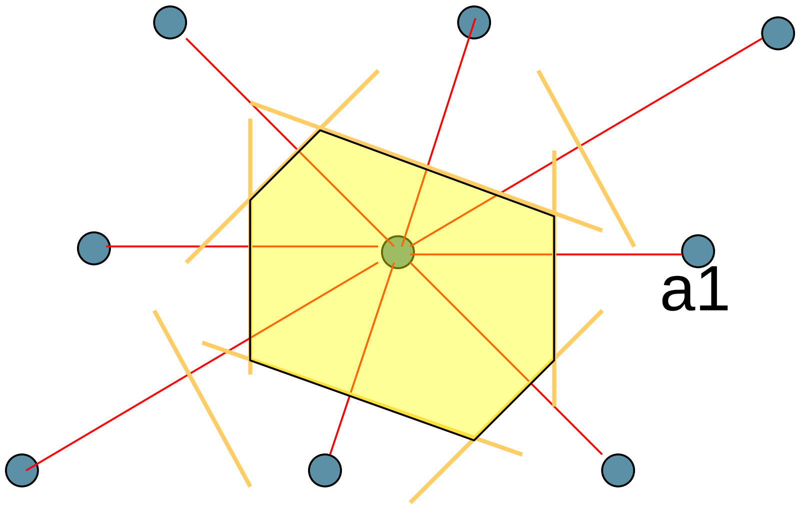
This is the full 3D Recipe!

Wigner Seitz algorithm
=> unit cell in reciprocal space

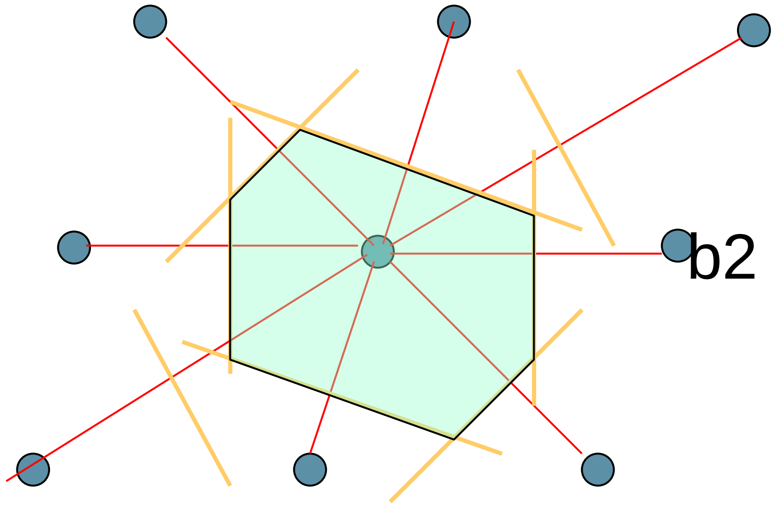


https://en.wikipedia.org/wiki/Reciprocal_lattice

Primitive cell in real space



Unit-cell in reciprocal lattice



Reciprocal Lattice of a Cube
Brillouin Zone in Cubic Lattice ...

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)}$$

$a_2 \times a_3 \parallel a_1$

$b_1 \parallel a_1$

$$b_2 = 2\pi \frac{a_3 \times a_1}{a_2 \cdot (a_3 \times a_1)}$$

$a_3 \times a_1 \parallel a_2$

$b_2 \parallel a_2$

$$b_3 = 2\pi \frac{a_1 \times a_2}{a_3 \cdot (a_1 \times a_2)}$$

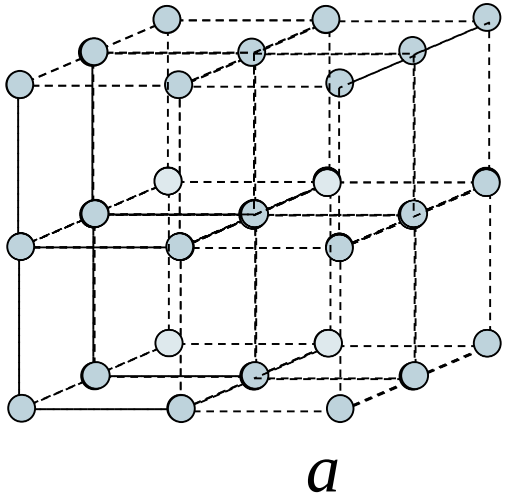
$a_1 \times a_2 \parallel a_3$

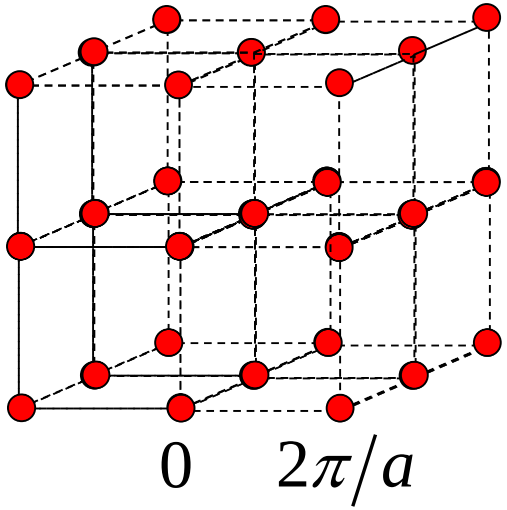
$b_3 \parallel a_3$

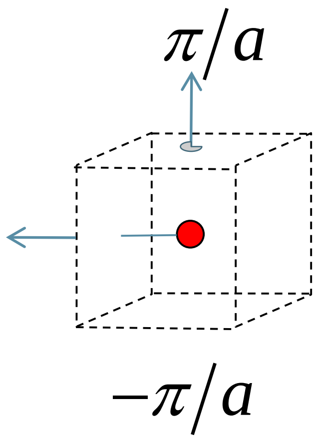
Real Space Cubic Lattice

Reciprocal Lattice

Brillouin Zone



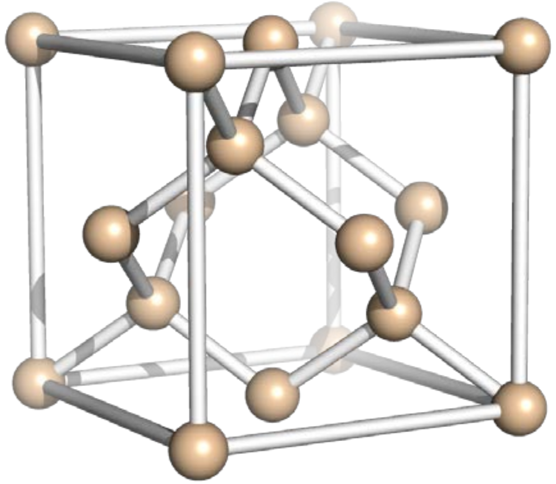




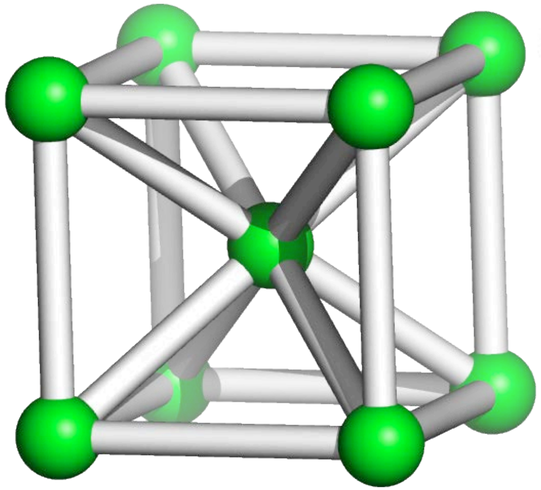
Follow W-S algorithm, but now for reciprocal lattice

Reciprocal Lattices and Brillouin Zone in *Real* FCC Lattices …

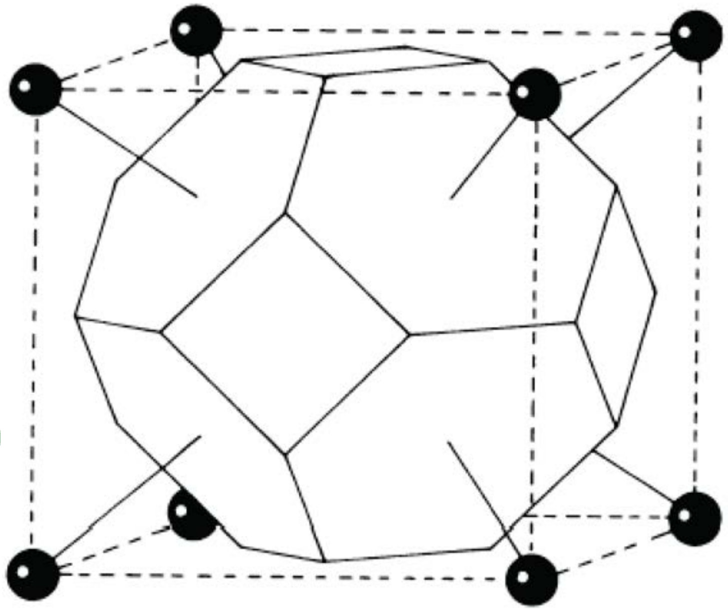
Real Space FCC (for Si, Ge, GaAs)



Reciprocal Lattice



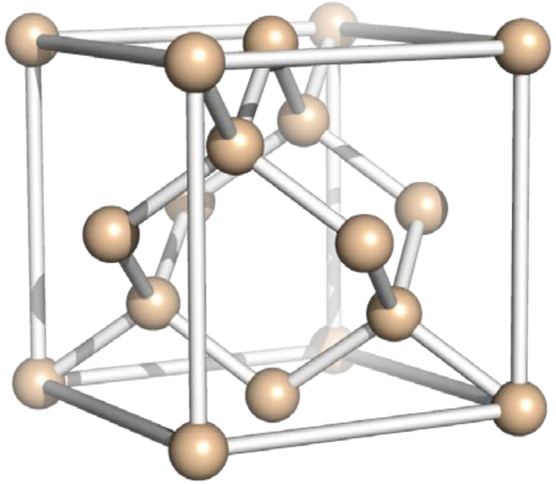
Brillouin Zone of Reciprocal Lattice



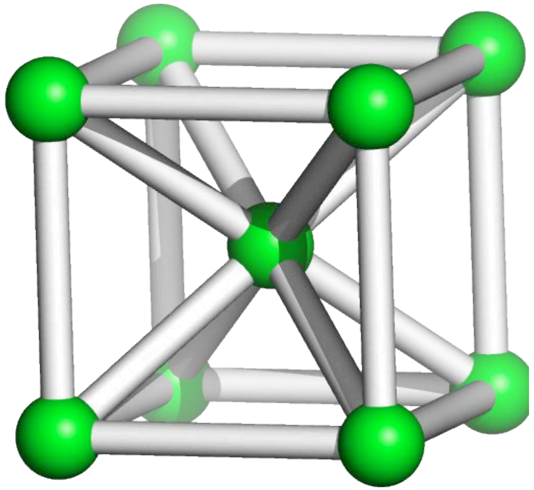
Diamond lattice and bcc are
Fourier Transforms of each other!

Brillouin Zone in *Real* FCC Lattices …

Real Space FCC (for Si, Ge, GaAs)

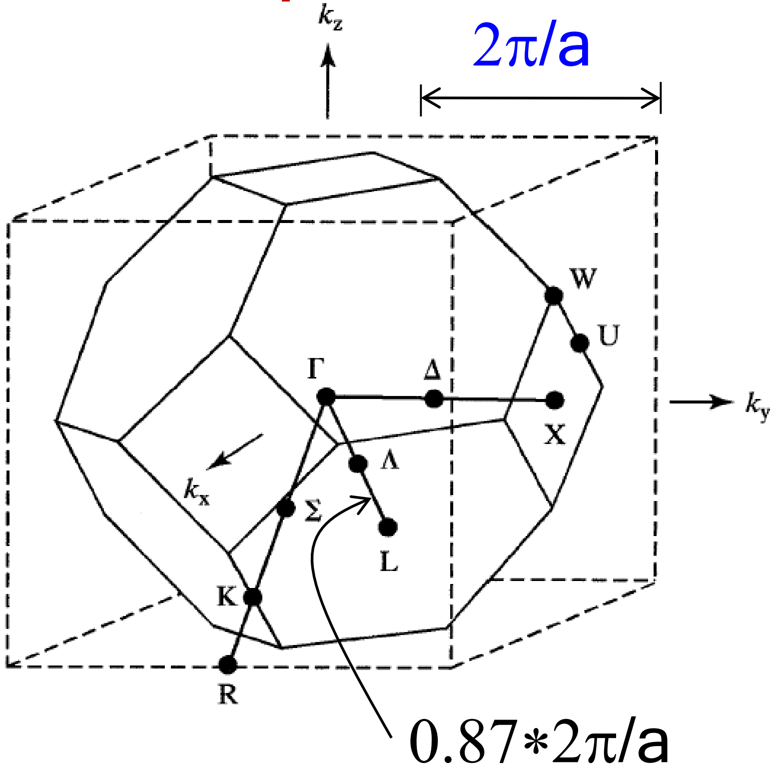


Reciprocal Lattice



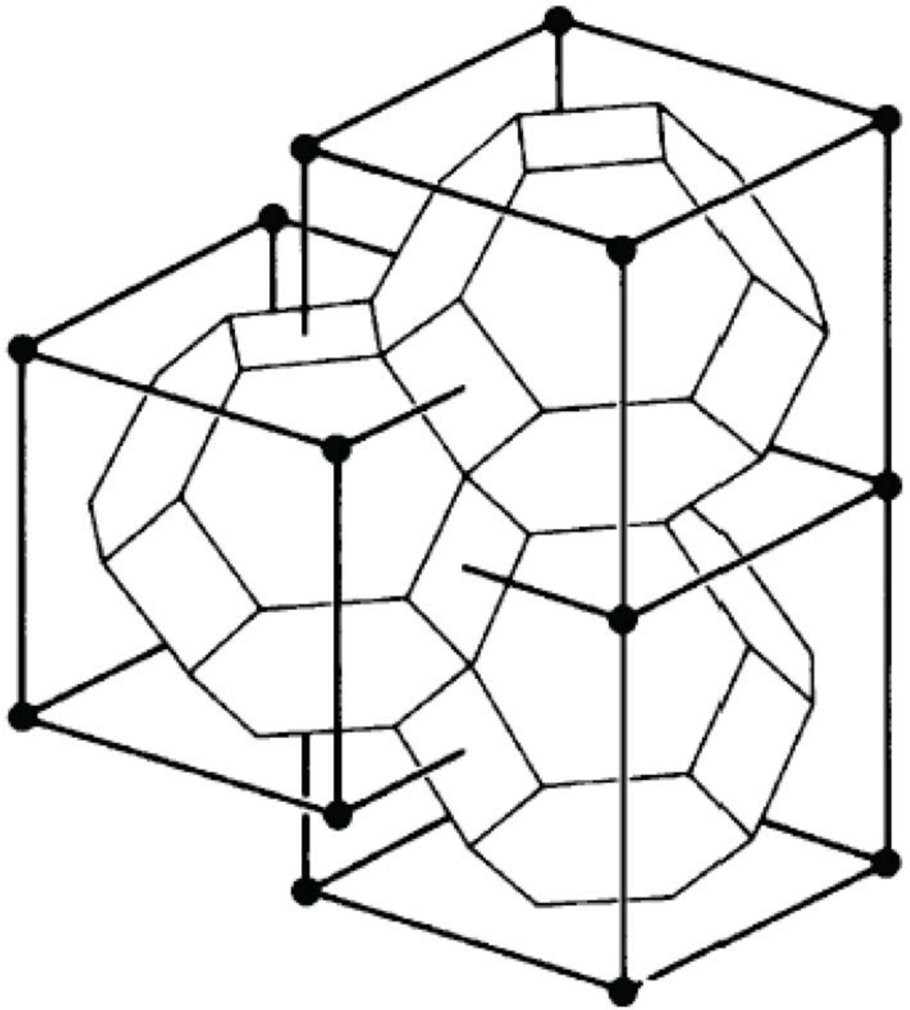
Diamond lattice and bcc are Fourier Transforms of each other!

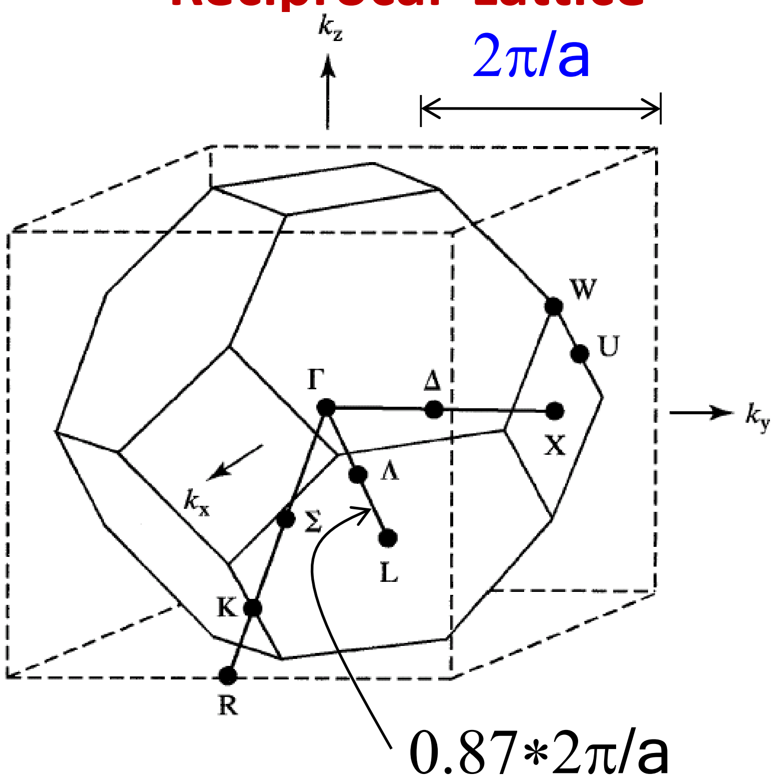
Brillouin Zone of Reciprocal Lattice



Note unlike cubic lattice, zone edge is not at π/a

Brillouine Zone is Space Filling



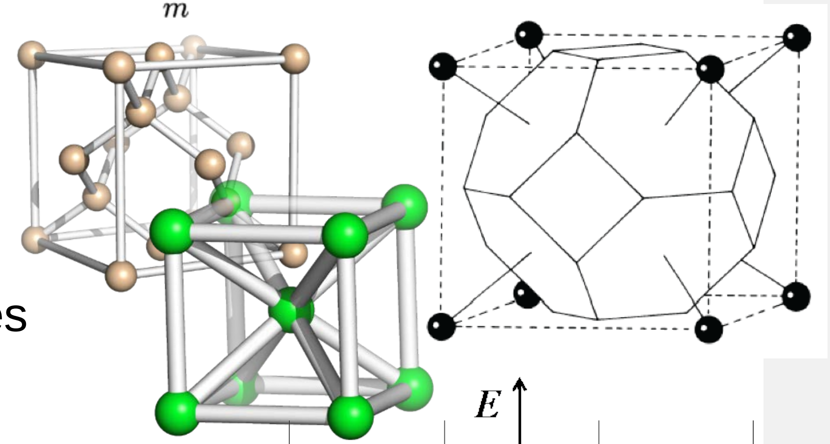


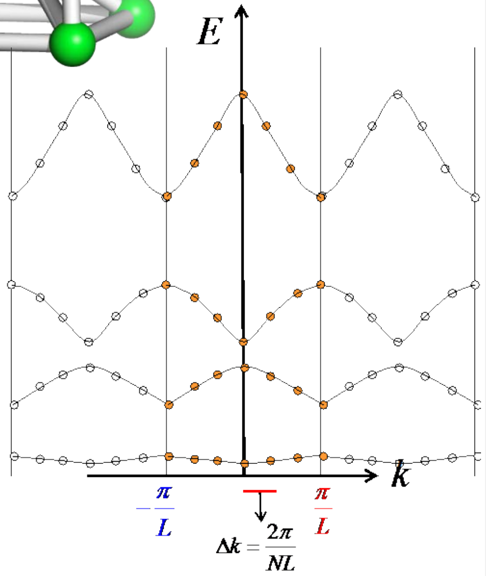
Note unlike cubic lattice, zone edge is not at π/a

- Basis State Selection
  - » Physical problem is based on a 1D/2D/3D periodic array of atoms
  - » Desired system/signal response is periodic in space
  - » Physical space is infinitely extended
    - ✓ Can the physical space be collapsed into a different representation?
  - » Chose a basis system of plane waves
  - » New finite reciprocal space is representative of the original system
  - » In 2D and 3D the reciprocal space may have critical axes/symmetries
- Solution of the Schrödinger Equation
  - » Solution with plane waves in reciprocal space
  - » 1D solution performed in Kronig-Penney model (last Section 7)
    - ✓ Band formation
  - » 2D/3D solution along critical paths in the reciprocal space (next Section 9)

$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$$

$$\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$$

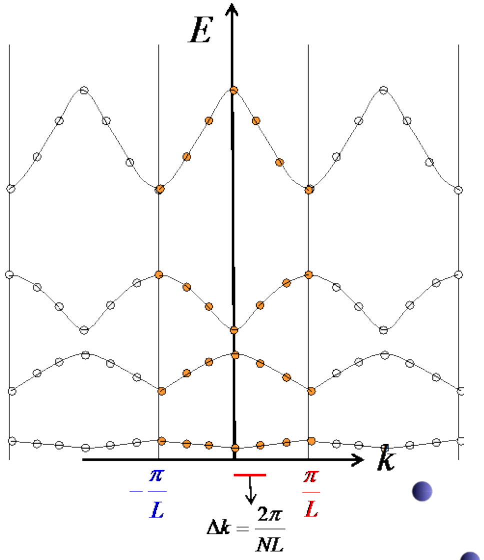




Section 8
Brillouin Zone and Reciprocal Lattice

One Video Segment

- 8.1 1D Problems
  - » Brillouin Zone
  - » Solution strategy
  - » Reciprocal Lattice

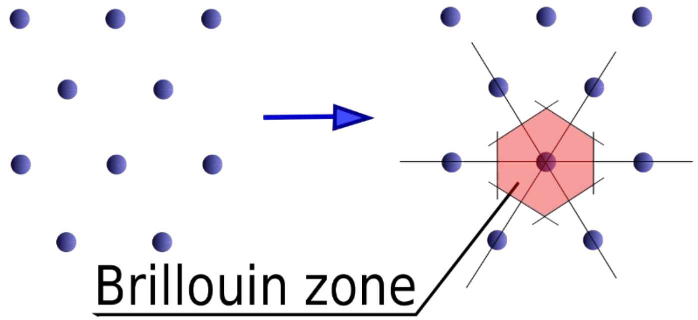


$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$$

$$\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$$

One Video Segment

- 8.2 2D Problems
  - » Reciprocal Lattice Recipe
  - » Examples - Square and Hexagonal



$$\boldsymbol{b}_1 = 2\pi \frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot \bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2}$$

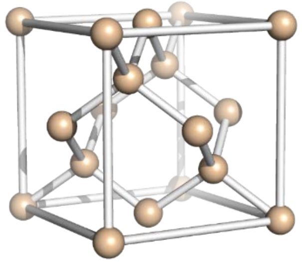
$$\boldsymbol{b}_2 = 2\pi \frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1}{\boldsymbol{a}_2 \cdot \bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1}$$

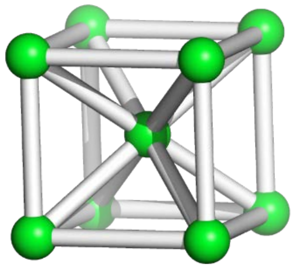
$$\cos\theta = \boldsymbol{a}_1 \cdot \boldsymbol{a}_2$$

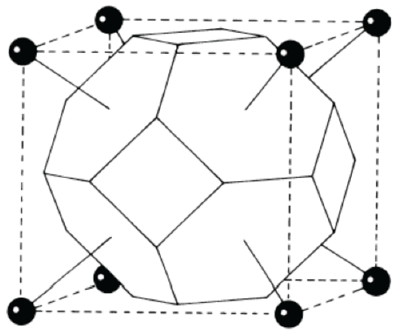
$$\bar{\bar{\boldsymbol{R}}} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

One Video Segment

- 8.3 3D Problems
  - » Reciprocal Lattice Recipe
  - » Examples







$$\boldsymbol{b}_1 = 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)}$$

$$\boldsymbol{b}_2 = 2\pi \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_2 \cdot (\boldsymbol{a}_3 \times \boldsymbol{a}_1)}$$

$$\boldsymbol{b}_3 = 2\pi \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\boldsymbol{a}_3 \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2)}$$

Prasad Sarangapani, Arun Goud Akkala, Sebastian Steiger, Hong-Hyun Park, Yosef Borga, Tillmann Christoph Kubis, Michael Povolotskyi, Gerhard Klimeck (2014), "Brillouin Zone Viewer," https://nanohub.org/resources/brillouin. (DOI: 10.4231/D3DB7VQ35).