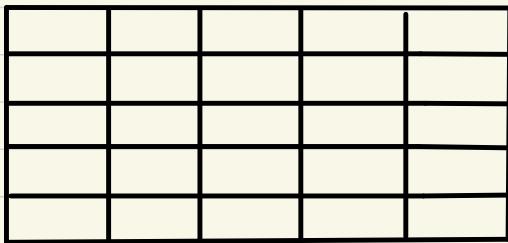


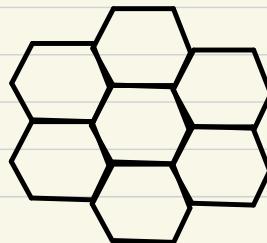
I.C: Crystal lattices (h and p ch. II)

- key feature of (crystalline) solids: Periodicity
- In 1D, periodicity is trivial
- What about 2D and 3D ??
- * Periodicity more complicated, but still have same concepts
- * Crystals described by lattice of points where one or more atoms are located at/around
- * There is a finite number of periodic lattices!
 - Why? Only certain shapes tessellate to fill space

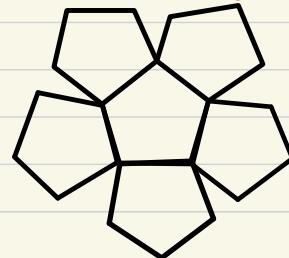
Squares / rectangles



Hexagons



NOT pentagons!



* Properties of crystals have the same periodicity and symmetry as the lattice (for the most part)

* "Reciprocal space" will play a significant role, as it did in 1D

- No longer just scalar $-\frac{\pi}{4} \leq k \leq \frac{\pi}{4}$, now have reciprocal lattice vectors

Bravais lattices

- Definition: regular periodic arrangement of points in space connected by translation vectors:

$$\vec{t}_n = n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3 \quad \in \mathbb{Z}$$

↑ ↑ ↑
Primitive/fundamental
translation vectors

- Primitive unit cell: parallelepiped formed by $\vec{t}_1, \vec{t}_2, \vec{t}_3$

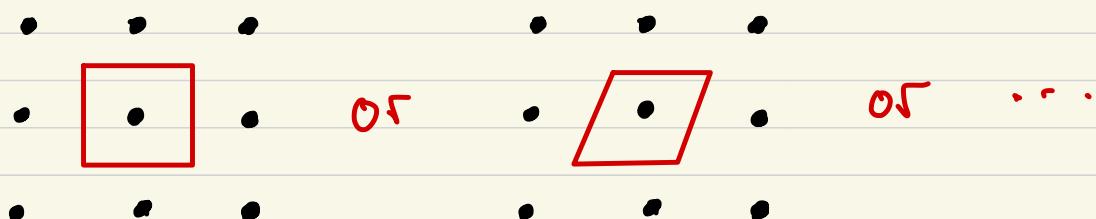
* Unit cell volume: $\Omega = \vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)$

* (order of vectors chosen to form "right hand" system)

* Contains one "lattice point"

* unit cell usually defined by cell lengths a, b, c and angles α, β, γ

* NOT UNIQUE! Infinite number of choices describing the same infinite lattice



- Can always define a 3×3 transformation matrix $M \rightarrow$ has unit determinant and integer values m_{ij} ($i, j = 1, 2, 3$)

Consider new triad of points

$$\vec{t}'_1 = m_{11} \vec{t}_1 + m_{12} \vec{t}_2 + m_{13} \vec{t}_3$$

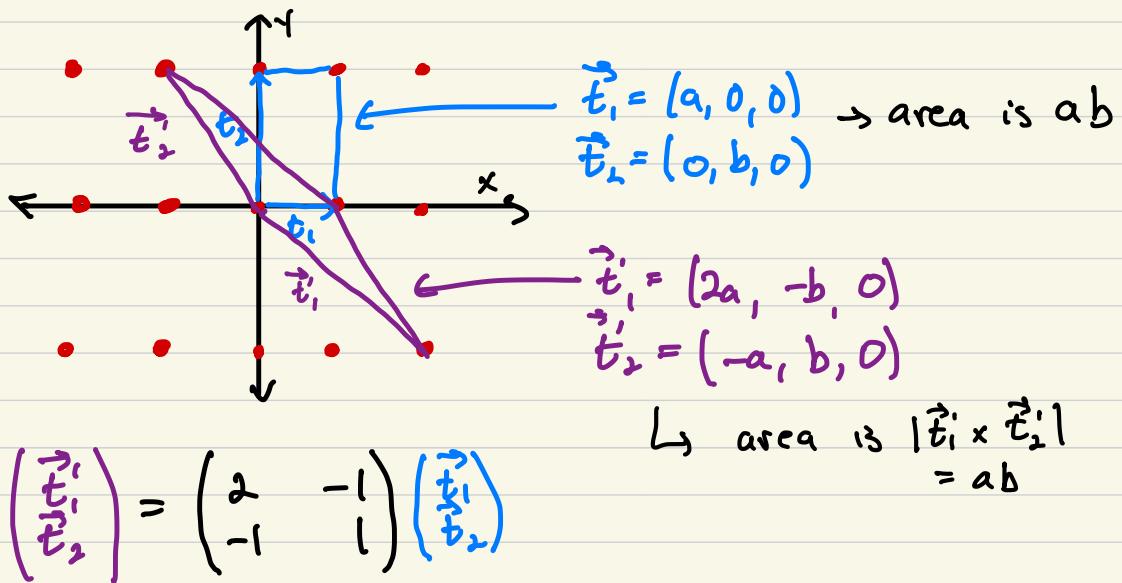
$$\vec{t}'_2 = m_{21} \vec{t}_1 + m_{22} \vec{t}_2 + m_{23} \vec{t}_3$$

$$\vec{t}'_3 = m_{31} \vec{t}_1 + m_{32} \vec{t}_2 + m_{33} \vec{t}_3$$

- Can show that set of points generated by $\vec{t}_1', \vec{t}_2', \vec{t}_3'$ are the same as $\vec{t}_1, \vec{t}_2, \vec{t}_3$

- Volume is the same since $\det M = 1$

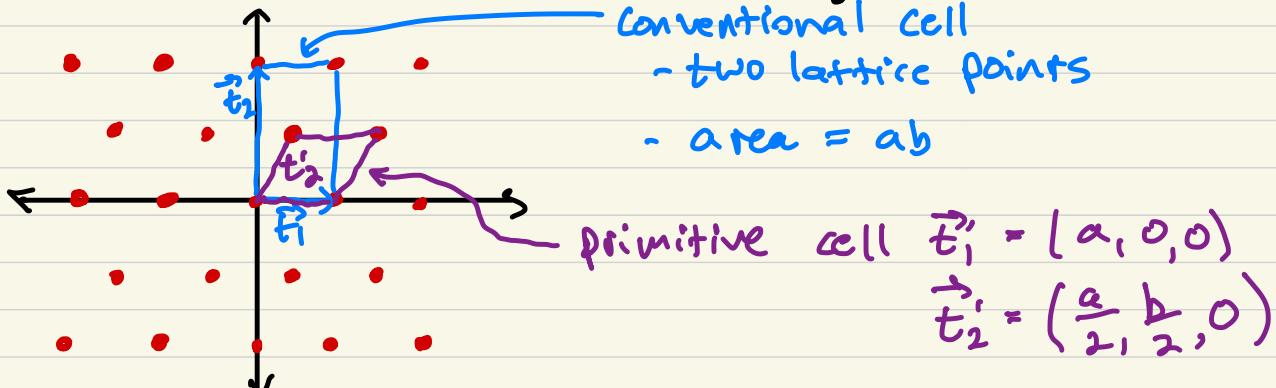
- Example:



- Sometimes it is useful to use non primitive cells that better illustrate the lattice

* Called "conventional unit cells"

* Consider 2D "centered" rectangular lattice

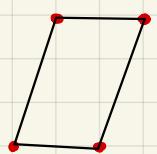


$$\begin{pmatrix} \vec{t}_1' \\ \vec{t}_2' \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} \vec{t}_1 \\ \vec{t}_2 \end{pmatrix}$$

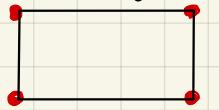
Note, $\det M \neq 1 !!$

- five possible Bravais lattices in 2D

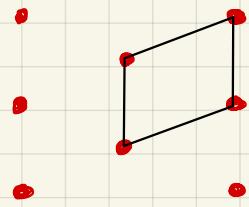
Obligee



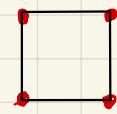
Primitive rectangular



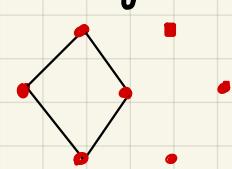
Centered rectangular



Square



hexagonal

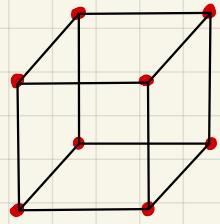


- 14 Bravais lattices in 3D

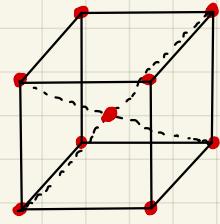
* Split into 7 "crystal systems"

- Cubic crystal system: $a = b = c$, $\alpha = \beta = \gamma = 90^\circ$

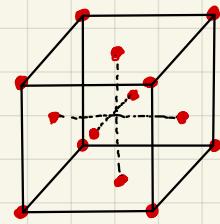
Primitive



Body-Centred

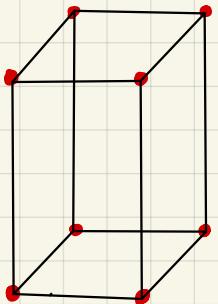


face-Centred

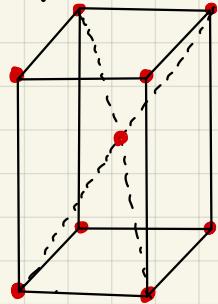


- Tetragonal: $a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$

Primitive

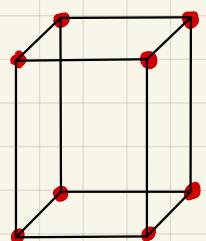


Body-centred

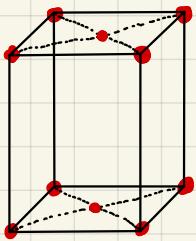


- Orthorhombic: $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$

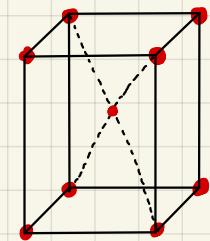
Primitive



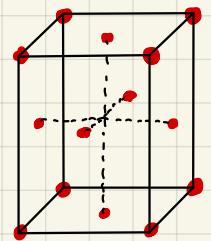
Base-centred



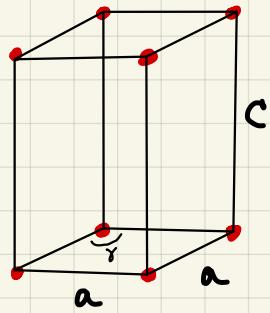
Body-centred



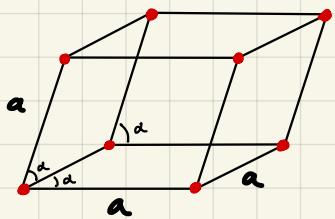
face-centred



- Hexagonal: (only primitive) $a=b \neq c$, $\alpha=\beta=90^\circ$ $\gamma=120^\circ$

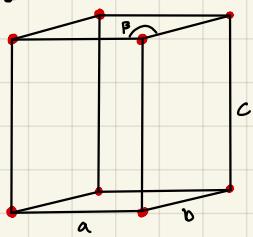


- Trigonal (only primitive): $a=b=c$, $\alpha=\beta=\gamma \neq 90^\circ$

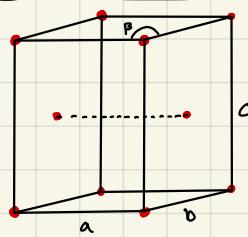


- Monoclinic: $a \neq b \neq c$, $\alpha=\gamma=90^\circ \neq \beta$

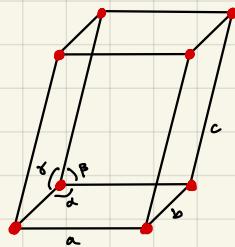
Primitive



Base - Centered



- Triclinic (only primitive): $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$



"Composite" crystals with a basis

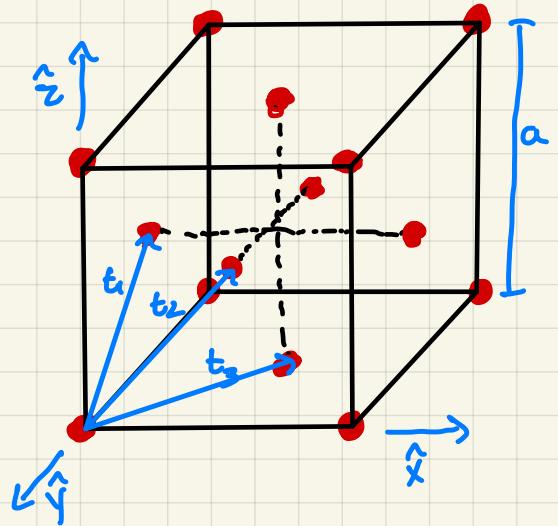
- Bravais lattice points given by $\vec{t}_1, \vec{t}_2, \vec{t}_3$
- At each lattice point there can be multiple atoms
 - * positions described by **basis vectors**
 - * Defined with respect to lattice points, but not given by primitive lattice vectors
 - * Can be the same element or different
- Complete crystal structure defined by:

$$\text{Crystal structure} = \left\{ \begin{array}{l} \vec{t}_1, \vec{t}_2, \vec{t}_3 \leftarrow \text{primitive translation vectors} \\ \vec{d}_1, \vec{d}_2, \dots, \vec{d}_v \leftarrow \text{basis vectors} \end{array} \right.$$

- Simple lattice: only atoms at lattice sites, no basis vectors
 - * Atomic positions: $\vec{R}_n = n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3$
- Composite lattice: two or more atoms in primitive cell
 - * Atomic positions:
 $\vec{R}_n^{(1)} = \vec{d}_1 + n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3$
 $\vec{R}_n^{(2)} = \vec{d}_2 + n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3$
 \vdots
 $\vec{R}_n^{(v)} = \vec{d}_v + n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3$

- * Composed of interpenetrating sublattices
 - All atoms in sublattice are the same
 - Different sublattices may or may not have different elements

- Example of simple lattice: face-centered cubic Al



* Atoms located at lattice points

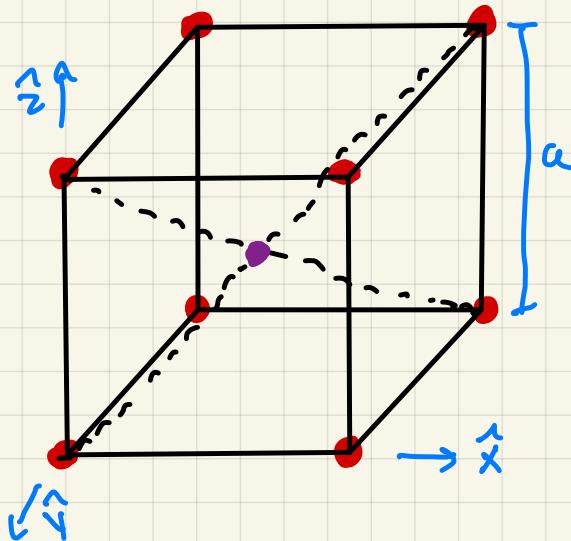
$$\vec{t}_1 = \frac{a}{2}(0, 1, 1)$$

$$\vec{t}_2 = \frac{a}{2}(1, 0, 1)$$

$$\vec{t}_3 = \frac{a}{2}(1, 1, 0)$$

* One sublattice so all atoms must be the same

- Example of composite lattice: CsCl structure



* looks like body-center cubic but with a different atom at the center

* Bravais lattice is simple cubic

$$\vec{t}_1 = a(1, 0, 0)$$

$$\vec{t}_2 = a(0, 1, 0)$$

$$\vec{t}_3 = a(0, 0, 1)$$

* Basis vectors (two sublattices):

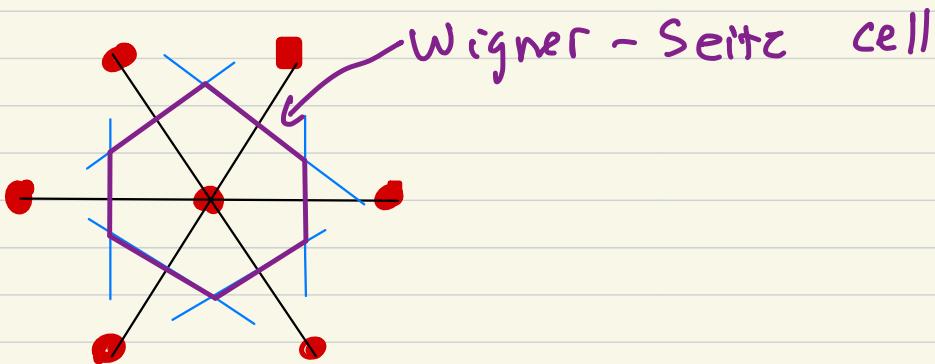
$$\vec{c}_1 = 0$$

$$\vec{c}_2 = \frac{a}{2}(1, 1, 1)$$

- See G and P Sec. II. 2 for many more examples!

Wigner - Seitz primitive cell

- We said before that the choice of primitive cell is not unique
 - * Actually infinite number of choices (by varying the origin)
 - One useful choice suggested by Wigner and Seitz
- * Definition: Consider a lattice point. The WS cell is the one where any point on the cell is closer to that lattice point than any other lattice point.
- * Construction: draw lines between lattice points and bisect them with lines (in 2D) or planes (3D).



* Properties:

- Primitive cell

- Constructed from underlying Bravais lattice if there is a basis
 - Has all of the symmetry of the Bravais lattice
- * I.e., most symmetric choice of primitive cell

Reciprocal Lattice

- We saw in 1D that it is useful to consider the electronic structure in reciprocal space
- How do we do this in 3D?

* Instead of one, we have three primitive reciprocal lattice vectors:

$$\vec{t}_i \cdot \vec{g}_j = 2\pi \delta_{ij} \quad \text{Convention}$$

real space \uparrow primitive lattice vectors $(\vec{t}_1, \vec{t}_2, \vec{t}_3)$
 \uparrow reciprocal lattice vectors $(\vec{g}_1, \vec{g}_2, \vec{g}_3)$

* As before, wavevectors k (e.g., for plane waves) defined in reciprocal space

* Reciprocal lattice points: $\vec{g}_m = m_1 \vec{g}_1 + m_2 \vec{g}_2 + m_3 \vec{g}_3$

* Only depends on real-space lattice vectors

- Same no matter the basis

* since $\vec{g}_1 \perp \vec{t}_2$ and $\vec{g}_1 \perp \vec{t}_3$, $\vec{g}_1 \parallel \vec{t}_2 \times \vec{t}_3$

$$\text{so: } \vec{g}_1 = \frac{2\pi}{\Omega} \vec{t}_2 \times \vec{t}_3 \text{ where } \Omega = \vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)$$

\hookrightarrow volume of primitive cell

- By cyclic permutations:

$$\vec{g}_2 = \frac{2\pi}{\Omega} \vec{t}_3 \times \vec{t}_1, \quad \vec{g}_3 = \frac{2\pi}{\Omega} \vec{t}_1 \times \vec{t}_2$$

* NOTE: Reciprocal lattice is a lattice of points in reciprocal space related to the real-space lattice vectors by the above relations

* Volume of unit cell in reciprocal space:

$$\begin{aligned}
 \Omega_K &= \vec{g}_1 \cdot (\vec{g}_2 \times \vec{g}_3) = \frac{(2\pi)^3}{\Omega^3} (\vec{t}_2 \times \vec{t}_3) \cdot [(\vec{t}_3 \times \vec{t}_1) \times (\vec{t}_1 \times \vec{t}_2)] \\
 &= \frac{(2\pi)^3}{\Omega^3} (\vec{t}_2 \times \vec{t}_3) \cdot [-(\vec{t}_1 \times \vec{t}_3) \times (\vec{t}_1 \times \vec{t}_2)] \\
 &= \frac{(2\pi)^3}{\Omega^3} (\vec{t}_2 \times \vec{t}_3) \cdot [-\vec{t}_1 \cdot (\vec{t}_3 \times \vec{t}_2)] \vec{t}_1 \stackrel{\substack{(a \times b) \times (a \times c) \\ = (a \cdot (b \times c)) a}}{=} \\
 &= \frac{(2\pi)^3}{\Omega^2} (\vec{t}_2 \times \vec{t}_3) \cdot \vec{t}_1 = \boxed{\frac{(2\pi)^3}{\Omega} = \Omega_K}
 \end{aligned}$$

* For arbitrary lattice point in real (t_n) and reciprocal (\vec{g}_n) space:

$$\vec{g}_m \cdot \vec{t}_n = 2\pi M \text{ where } M \in \mathbb{Z}$$

* If vector \vec{q} satisfies $\vec{q} \cdot \vec{t}_n = 2\pi M$ for any \vec{t}_n , it is a reciprocal lattice vector

- why? Can write $\vec{q} = c_1 \vec{g}_1 + c_2 \vec{g}_2 + c_3 \vec{g}_3$
 $\vec{t}_n = d_1 \vec{t}_1 + d_2 \vec{t}_2 + d_3 \vec{t}_3$
 $c_1, c_2, c_3 \in \mathbb{Z}$

$$\therefore \vec{q} \cdot \vec{t}_n = 2\pi (c_1 d_1 + c_2 d_2 + c_3 d_3)$$

$$= 2\pi M \text{ if } c_1, c_2, c_3 \in \mathbb{Z}$$

but integer multiples of $(\vec{g}_1, \vec{g}_2, \vec{g}_3)$ is the definition of reciprocal lattice vectors

- This implies that a plane wave $e^{i\vec{k} \cdot \vec{r}}$ has the periodicity of the lattice iff \vec{k} is a reciprocal lattice vector

Consider $w(\vec{r}) = e^{i\vec{g}_m \cdot \vec{r}}$

$$w(\vec{r} + \vec{t}_n) = e^{i\vec{g}_m \cdot \vec{r}} e^{i\vec{g}_m \cdot \vec{t}_n} = e^{i\vec{g}_m \cdot \vec{r}} e^{2\pi i M} \quad \boxed{m \in \mathbb{Z}}$$

$$= w(\vec{r})$$

- Thus if $f(r)$ has the periodicity of the lattice:

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

and if $F(k)$ has the periodicity of the reciprocal lattice:

$$F(k) = \sum_m F_m e^{i\vec{k} \cdot \vec{t}_m}$$

- This is the generalization to 3D of the discussion of the 1D Fourier transform of the periodic potential that led us to Bloch's theorem

Planes and directions in Bravais lattices

- Recall: Bravais lattice defined by points connected by translation vectors:

$$\vec{t}_n = n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3$$

- $n_1, n_2, n_3 \in \mathbb{Z}$
- $\vec{t}_1, \vec{t}_2, \vec{t}_3$ are prim. translation vectors

- We can use reciprocal lattice vectors to define 2D planes in real space on which all lattice points fall

- Consider reciprocal lattice vector with minimum length in a given direction.

* Implies that if $\vec{g}_m = m_1 \vec{g}_1 + m_2 \vec{g}_2 + m_3 \vec{g}_3$

then m_1, m_2, m_3 have no common divisors

* The scalar product of \vec{g}_m with any \vec{t}_n is:

$$\vec{g}_m \cdot \vec{t}_n = 0, \pm 2\pi, \pm 4\pi, \pm 6\pi, \dots$$

• Why? if $\vec{g}_m \cdot \vec{t}_n = 0, \pm 2\pi, \pm 4\pi, \dots$ with $\gamma > 1$, then \vec{g}_m/γ would also be a reciprocal lattice vector and m_1, m_2, m_3 would have a common divisor

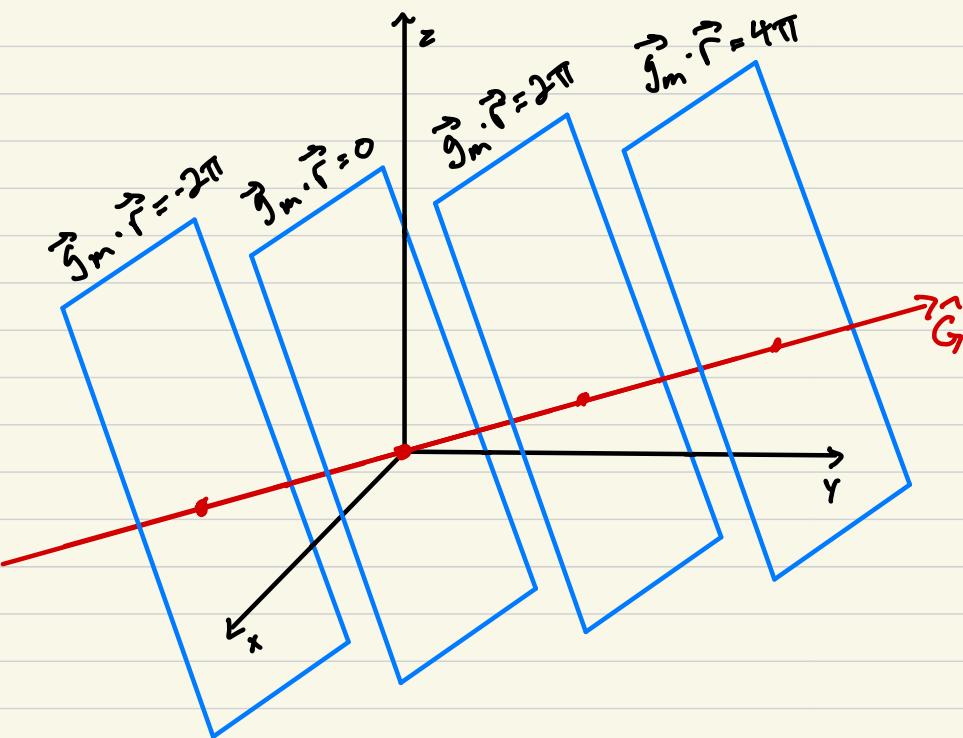
* Therefore: all translation vectors in real space belong to equidistant planes perpendicular to \vec{g}_m separated by:

$$d = \frac{2\pi}{|\vec{g}_m|}$$

• We will return to this when discussing diffraction

• thus lattice points fall on these 2D planes (see next page)

- Lattice planes defined by \vec{g}_m :



- We denote this family of planes (m_1, m_2, m_3)

* Note that there may be several families of planes that are equivalent by symmetry

- For example in a cube, all faces are symmetrically equivalent, so $(0,0,1)$, $(0,1,0)$, $(1,0,0)$ are equivalent

- Denote set of sym. equivalent families of planes as $\{m_1, m_2, m_3\}$

- E.g., for cubic $\{1,0,0\} \rightarrow [0,0,1], [0,1,0], [1,0,0]$

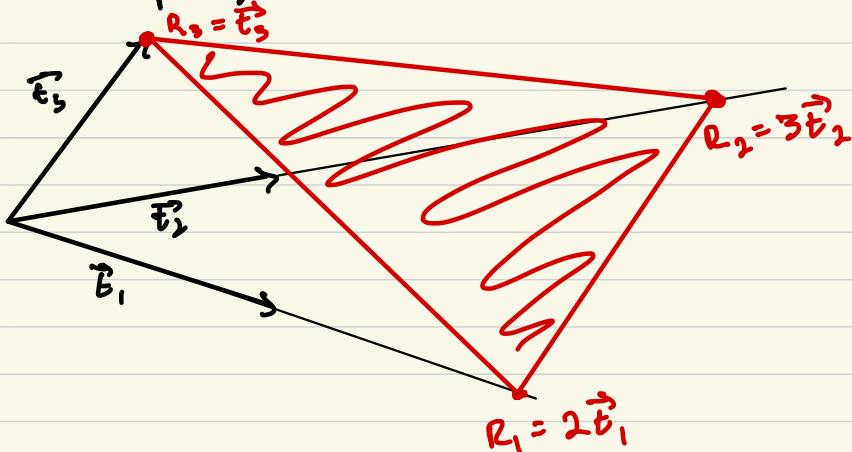
- Alternative (equivalent) way of defining / constructing these planes: Miller indices

* Consider plane given by 3 non collinear lattice points

* Take the inverse of the intercepts with the primitive lattice vectors $\vec{t}_1, \vec{t}_2, \vec{t}_3$

* multiply by smallest factor to get three integers

- Example:



* Intercepts: $\vec{R}_1 = 2\vec{t}_1$, $\vec{R}_2 = 3\vec{t}_2$, $\vec{R}_3 = \vec{t}_3$

inverses: $\frac{1}{2}, \frac{1}{3}, 1$

make integers: $\left(\frac{1}{2}, \frac{1}{3}, 1\right) * 6 = (3, 2, 6)$ ← Miller indices of plane

* Consider reciprocal lattice vector: $\vec{g}_m = 3\vec{g}_1 + 2\vec{g}_2 + 6\vec{g}_3$

$$\bullet \vec{g}_m \cdot \vec{R}_1 = 12\pi, \vec{g}_m \cdot \vec{R}_2 = 12\pi, \vec{g}_m \cdot \vec{R}_3 = 12\pi$$

⇒ Thus \vec{g}_m is perpendicular to $\vec{R}_1 - \vec{R}_2$ and $\vec{R}_2 - \vec{R}_3$

⇒ Thus \vec{g}_m is perpendicular to the lattice plane!

* Miller indices of plane equivalent to reciprocal lattice vector perpendicular to it.

- Crystallographic directions between lattice points:

* Write vector connecting two lattice points as

$$\vec{t}_n = n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3$$

* divide n_1, n_2, n_3 by highest common factor to get l_1, l_2, l_3

* Notation for direction is $[l_1, l_2, l_3]$

* Including sym. equivalent directions: $\langle l_1, l_2, l_3 \rangle$

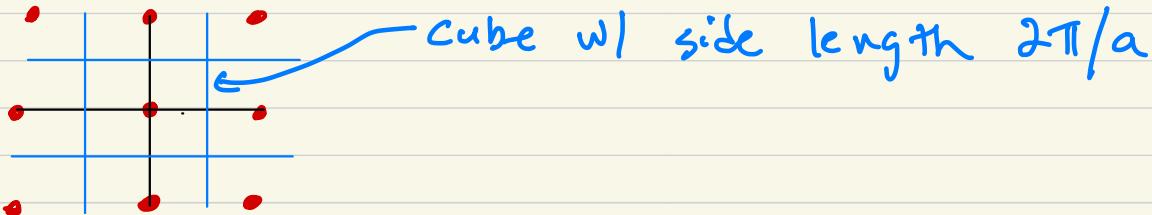
The Brillouin Zone in 3D crystals

- Definition: The first Brillouin zone is the Wigner - Seitz cell of the reciprocal lattice
- * Only depends on the geometry of the Bravais lattice, does not depend on the basis
- For some Bravais lattices, the real - and reciprocal - space lattices have the same shape (e.g., simple cubic and hexagonal)
- * Consider the example of simple cubic:

$$\vec{t}_1 = a(1, 0, 0) \quad \vec{t}_2 = a(0, 1, 0) \quad \vec{t}_3 = a(0, 0, 1)$$

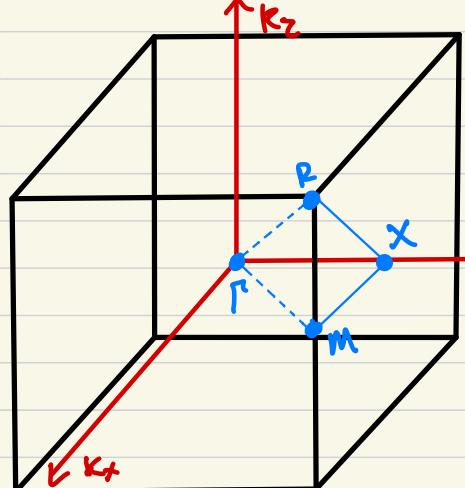
$$\vec{g}_1 = \frac{2\pi}{a}(1, 0, 0) \quad \vec{g}_2 = \frac{2\pi}{a}(0, 1, 0) \quad \vec{g}_3 = \frac{2\pi}{a}(0, 0, 1)$$

- For a square, the WS construction is trivial:



- How would we plot the electronic bands in a 3D Brillouin zone?

⇒ Define "high-symmetry" points, connect them with lines, plot along lines.



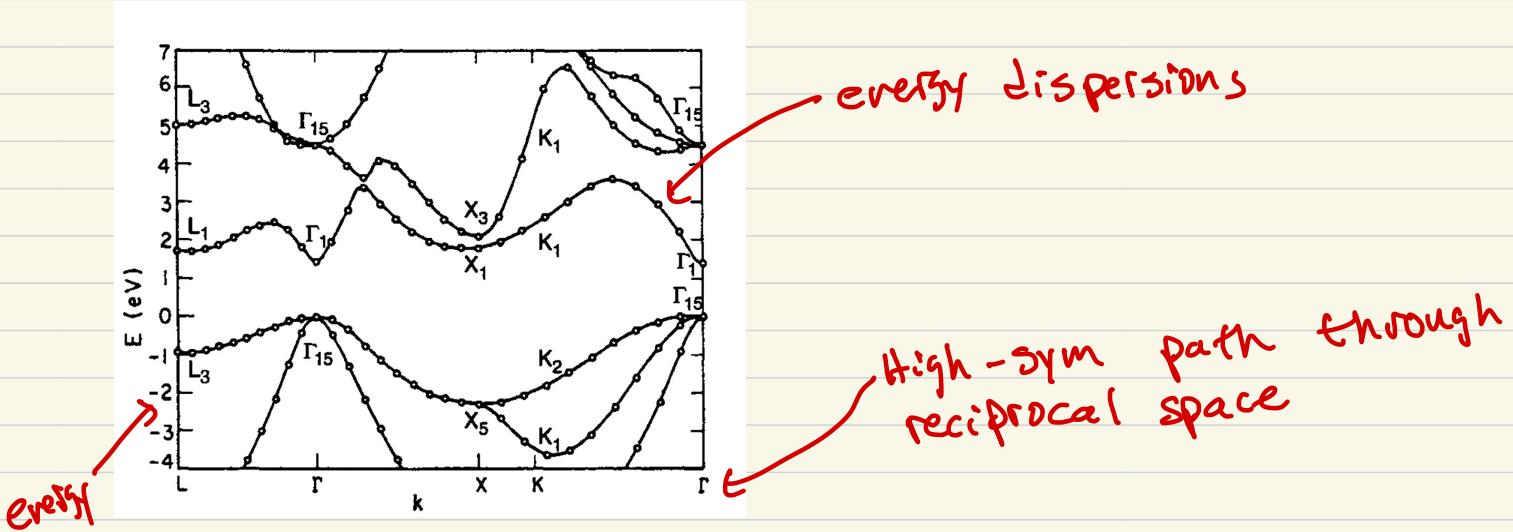
$$\Gamma = (0, 0, 0) \rightarrow \text{always called } \Gamma$$

$$X = \frac{2\pi}{a}(0, \frac{1}{2}, 0)$$

$$M = \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2}, 0)$$

$$R = \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$$

- For example (see G and P pg. 165):



- Why?
 - ⇒ often important elements of the dispersion (e.g. extrema) are at high-symmetry points
 - ⇒ Gives a sense of properties along different symmetry - inequivalent directions in a crystal
- Most Bravais lattices have different shapes for the real- and reciprocal-space lattices
 - * See G and P Sec. II.5 for many examples

Electronic structure and dynamics in 3D crystals

- We have already discussed the effect of periodicity in 1D
- * Many concepts and formalism apply also to 3D
- Recall: $V(\vec{r})$ having the periodicity of the lattice means that we can write:

$$V(r) = \sum_{\vec{g}_m} V(\vec{g}_m) e^{i \vec{g}_m \cdot \vec{r}}$$

* Now apply $V(r)$ to plane waves: $W_k(\vec{r}) = \frac{1}{\sqrt{N\Omega}} e^{i \vec{k} \cdot \vec{r}}$

$$\langle W_k | V | W_{k'} \rangle = \int d^3 r \int d^3 r' \langle W_k | r \rangle \langle r | V | r' \rangle \langle r' | W_{k'} \rangle$$

$V(r)$ is diagonal in real space, i.e. $\langle r | V | r' \rangle = V(r) \delta(r - r')$

$$\begin{aligned} &= \frac{1}{N\Omega} \sum_{\vec{g}_m} V(\vec{g}_m) \int_{\text{crystal}} e^{i(-\vec{k}' + \vec{k} + \vec{g}_m) \cdot \vec{r}} d^3 r \\ &= \begin{cases} 0 & \text{if } \vec{k}' \neq \vec{k} + \vec{g}_m \\ V(\vec{k}' - \vec{k}) & \text{if } \vec{k}' = \vec{k} + \vec{g}_m \end{cases} \end{aligned}$$

- Therefore, if \vec{k} and \vec{k}' are both in the first BZ, the periodic potential does not mix them

- Thus, we can write:

$$\begin{aligned} \Psi_{\vec{k}}(\vec{r}) &= \sum_{\vec{g}_n} a_n(\vec{k}) e^{i(\vec{k} + \vec{g}_n) \cdot \vec{r}} \\ \Rightarrow \Psi_{\vec{k}}(\vec{r}) &= e^{i \vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r}) \end{aligned}$$

itinerant plane wave ↑ *cell periodic part*

- * As before we can plot $E(\vec{k})$ in first BZ, will be bands of allowed energies separated by gaps

- * As before, $\hbar \vec{k}$ is "crystal momentum" of e^-

k -points in 3D

- In 1D, when we considered Born-Von Karman boundary conditions we found that:

$$k = \frac{2\pi n}{Na} \quad n \in \mathbb{Z}, \quad N \text{ is number of repeat units of length } a$$

- In 3D, Br. k. B.C.s require:

$$\Psi(\vec{r}) = \Psi(\vec{r} + N_1 \vec{t}_1) = \Psi(\vec{r} + N_2 \vec{t}_2) = \Psi(\vec{r} + N_3 \vec{t}_3)$$

↑ # repeat units in dir 1 ↑ # repeat units in dir 2 ↑ # repeat units in dir 3

* If Ψ is a Bloch function with wavevector \vec{k} ,

$$\Psi_{\vec{k}}(\vec{r} + N_1 \vec{t}_1) = u_k(\vec{r} + N_1 \vec{t}_1) e^{i\vec{k}(\vec{r} + N_1 \vec{t}_1)} = \Psi_{\vec{k}}(\vec{r}) e^{i\vec{k} \cdot N_1 \vec{t}_1}$$

- Need to have: $e^{i\vec{k} \cdot N_1 \vec{t}_1} = e^{i\vec{k} \cdot N_2 \vec{t}_2} = e^{i\vec{k} \cdot N_3 \vec{t}_3} = 1$

- Compatible \vec{k} vectors are:

$$k = \frac{m_1}{N_1} \vec{g}_1 + \frac{m_2}{N_2} \vec{g}_2 + \frac{m_3}{N_3} \vec{g}_3 ; \quad m_1, m_2, m_3 \in \mathbb{Z}$$

- \vec{k} inside first Brillouin zone are given by choosing $0 \leq m_i < N_i$

- Thus $\underbrace{N_1 \cdot N_2 \cdot N_3}_{\text{\# of primitive cells in the crystal}} \vec{k}$ in 1st BZ.

of primitive cells in the crystal

- Density of \vec{k} in reciprocal space:

$$W(\vec{k}) = \frac{1}{\frac{1}{N_1} \vec{g}_1 \cdot \left(\frac{1}{N_2} \vec{g}_2 \times \frac{1}{N_3} \vec{g}_3 \right)} = \frac{N_1 N_2 N_3}{V_k} = \frac{V}{(2\pi)^3}$$

Volume of crystal
 Unit cell in reciprocal space

- $\sum_{\vec{k}} f(\vec{k}) \rightarrow \frac{V}{(2\pi)^3} \int f(\vec{k}) d\vec{k}$

- Semi-classical relations we had in 1D apply in 3D (just add vectors \vec{k}):

$$*\langle \Psi_{n\vec{k}} | \frac{\vec{p}}{m} | \Psi_{n\vec{k}} \rangle = \frac{1}{\hbar} \frac{\partial E_{n\vec{k}}}{\partial \vec{k}}$$

* for $m \neq n$:

$$\langle \Psi_{m\vec{k}} | \frac{\hbar \vec{p}}{m} | \Psi_{n\vec{k}} \rangle = - (E_{m\vec{k}} - E_{n\vec{k}}) \langle u_{m\vec{k}} | \frac{\partial}{\partial \vec{k}} | u_{n\vec{k}} \rangle$$

$$\langle u_{m\vec{k}} | \vec{p} | u_{n\vec{k}} \rangle = i \langle u_{m\vec{k}} | \frac{\partial}{\partial \vec{k}} u_{n\vec{k}} \rangle$$

* Recall our k.p expansion to second order in 1D:

$$E_{n\vec{k}} = E_{n\vec{k}_0} + \frac{\hbar^2 (k - k_0)^2}{2 m^*}$$

$$\text{where } \frac{m}{m^*} = 1 + \frac{1}{m} \sum_{n' \neq n} \frac{\langle \Psi_{n\vec{k}_0} | \vec{p} | \Psi_{n'\vec{k}_0} \rangle \langle \Psi_{n'\vec{k}_0} | \vec{p} | \Psi_{n\vec{k}_0} \rangle}{E_{n\vec{k}_0} - E_{n'\vec{k}_0}}$$

- In 3D:

$$E_{n\vec{k}} = E_{n\vec{k}_0} + \sum_{\alpha\beta} \frac{\hbar^2}{2m} \left(\frac{m}{m^*} \right)_{\alpha\beta} (\vec{k} - \vec{k}_0)_\alpha (\vec{k} - \vec{k}_0)_\beta$$

$$\text{where } \left(\frac{m}{m^*} \right)_{\alpha\beta} = \delta_{\alpha\beta} + \frac{1}{m} \sum_{n' \neq n} \frac{\langle \Psi_{n\vec{k}_0} | \vec{p}_\alpha | \Psi_{n'\vec{k}_0} \rangle \langle \Psi_{n'\vec{k}_0} | \vec{p}_\beta | \Psi_{n\vec{k}_0} \rangle}{E_{n\vec{k}_0} - E_{n'\vec{k}_0}}$$

Crystal lattices: What have we learned?

- Periodicity is more complicated in 3D!

- Finite number of periodic lattices in 2D and 3D

* Called Bravais lattices, defined by lattice points:

$$\vec{t}_h = n_1 \vec{t}_1 + n_2 \vec{t}_2 + n_3 \vec{t}_3, \quad n_1, n_2, n_3 \in \mathbb{Z}$$

$\hookrightarrow \vec{t}_1, \vec{t}_2, \vec{t}_3$ are primitive lattice vectors

* 5 lattices in 2D, 14 Bravais lattices in 3D

* Smallest repeating unit cell in 2D/3D called the primitive cell

- not unique! Infinite number of choices

- Contains one lattice point

- Wigner - Seitz construction gives one choice with full symmetry of the crystal

- Atomic positions in crystal given by lattice vectors in simple lattices, and lattice vectors + basis vectors in composite lattices:

$$\vec{r}_i = b_i + n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3$$

\hookrightarrow "sublattice" i

- Reciprocal lattice in 2D and 3D defined by reciprocal lattice points:

$$\vec{g}_m = m_1 \vec{g}_1 + m_2 \vec{g}_2 + m_3 \vec{g}_3 \quad m_1, m_2, m_3 \in \mathbb{Z}$$

$$\hookrightarrow \vec{g}_1 = \frac{2\pi}{V_{cell}} \vec{t}_2 \times \vec{t}_3, \quad \vec{g}_2 = \frac{2\pi}{V_{cell}} \vec{t}_3 \times \vec{t}_1, \quad \vec{g}_3 = \frac{2\pi}{V_{cell}} \vec{t}_1 \times \vec{t}_2$$

Volume of
real-space
primitive cell

primitive reciprocal lattice vectors

* Volume of primitive cell in reciprocal space: $\frac{(2\pi)^3}{V_{\text{cell}}}$

* Plane waves that have the periodicity of the lattice have k 's that are reciprocal lattice vectors

- If $f(r)$ is periodic w/ the lattice: $f(r) = \sum_m f_m e^{i\vec{g}_m \cdot \vec{r}}$
- Bloch's theorem in 3D: $\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r})$

* First Brillouin zone: Wigner - Seitz cell of reciprocal lattice

- plot bands along "high-symmetry lines" in BZ
- semiclassical relations generalize trivially to 3D
- Effective mass becomes a 3×3 matrix