

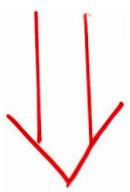
# (Direct) Bravais lattice (BL)

$\{\vec{a}_i\}$

primitive  
vectors

$$\vec{R} = \sum_i n_i \vec{a}_i$$

translations

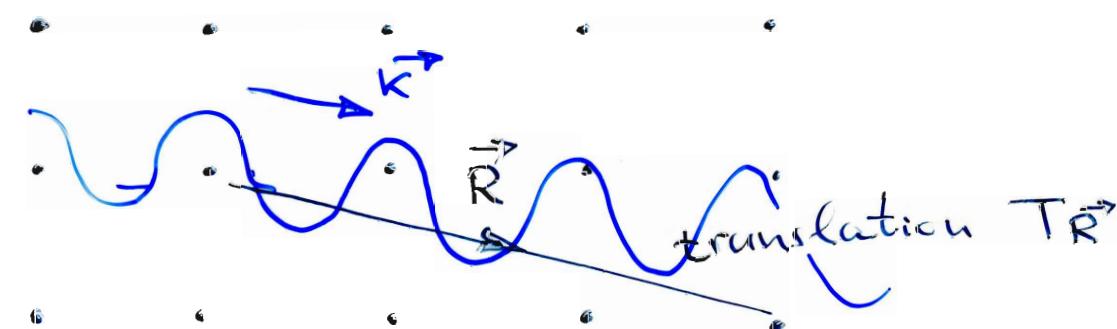


## Reciprocal lattice (RL)

Motivation:

- ① Classification of electron states  
in crystals allowed momenta  $\vec{k}$ ?
- ② Propagation and diffraction  
of waves (X-ray...) in crystals

Plane waves  $\exp(i\vec{k}\cdot\vec{r})$



$$T_{\vec{R}} e^{i\vec{k}\cdot\vec{r}} = e^{i\vec{k}\cdot(\vec{r} + \vec{R})} \neq e^{i\vec{k}\cdot\vec{r}}$$

GENERALLY  
because  $\exp(i\vec{k}\cdot\vec{R}) \neq 1$

RL: A special set of  $\vec{K}$ :  $\{\vec{K}\}$

$$\exp(i\vec{K} \cdot \vec{R}) = 1$$

$$\forall \vec{K} \text{ and } \forall \vec{R}$$

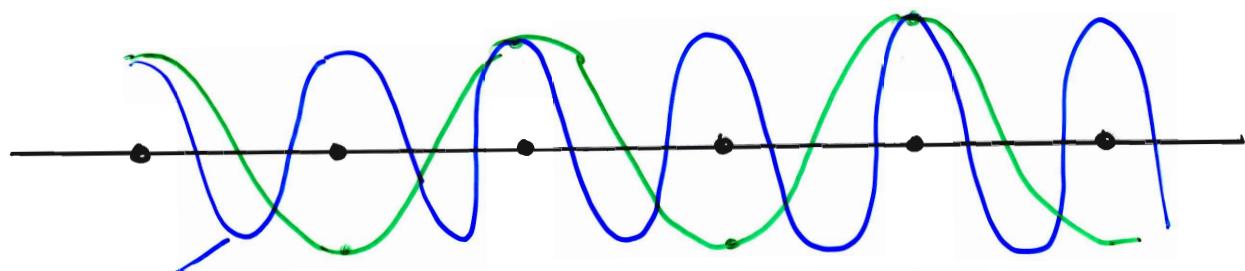
$\vec{R} \in BL$  that is  $\vec{R} = \sum_i n_i \vec{a}_i$

$$n_i = 0, \pm 1, \pm 2, \pm 3, \dots$$

### 1D example

$$\leftarrow a \rightarrow$$

$$R_1 = a \quad R_2 = 2a \quad R_3 = \dots$$



$$\text{wave number } k_1 = \frac{2\pi}{R_1} = \frac{2\pi}{a}$$

$$k_2 = \frac{2\pi}{R_2} = \frac{2\pi}{2a}$$

$$\text{wavelength } \lambda_1 = \frac{2\pi}{k_1} = a$$

$$\lambda_2 = \frac{2\pi}{k_2} = 2a$$

$\exists \infty$  number of discrete  $\vec{k}_i$

that are compatible with translations

RL is the set of all wave vectors  $\vec{K}$  that yield plane waves with the periodicity of the (direct) Bravais lattice

From analytic definition of RL

$$e^{i\vec{k} \cdot (\vec{r} + \vec{R})} = e^{i\vec{k} \cdot \vec{r}} \cdot e^{i\vec{k} \cdot \vec{R}} = e^{i\vec{k} \cdot \vec{r}}$$

$$\boxed{e^{i\vec{k} \cdot \vec{R}} = 1} \Leftrightarrow \vec{k} \cdot \vec{R} = 2\pi \cdot m \quad m=0, \pm 1, \pm 2, \dots$$

$$\forall \vec{R} = \sum_i n_i \vec{\alpha}_i \in \text{direct BL}$$

Theorem I. RL is a BL itself

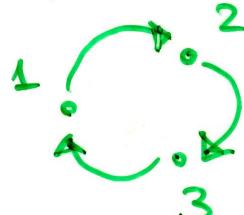
Constructive proof: RL can be generated by the three primitive vectors as a BL!

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

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

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

cyclic permutations



Note 1.  $\vec{\alpha}_1 \cdot (\vec{\alpha}_2 \times \vec{\alpha}_3) = (\vec{\alpha}_1 \times \vec{\alpha}_2) \cdot \vec{\alpha}_3 = \vec{\alpha}_2 \cdot (\vec{\alpha}_3 \times \vec{\alpha}_1)$

2.  $|\vec{\alpha}_1 \cdot (\vec{\alpha}_2 \times \vec{\alpha}_3)| = V$  volume of the primitive cell

Properties of  $\{\vec{a}_i\}$   $\{\vec{b}_j\}$

$$\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij} = \begin{cases} 2\pi & i=j \\ 0 & i \neq j \end{cases}$$

Kronecker  
delta

E.g.  $\vec{a}_1 \cdot \vec{b}_1 = \vec{a}_1 \cdot 2\pi \cdot \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi$

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

$$\vec{a}_1 \cdot (\vec{a}_3 \times \vec{a}_1) = 0$$

orthogonal

Now

$$\vec{K} = \sum_{j=1}^3 m_j \vec{b}_j$$

$$\vec{R} = \sum_{i=1}^3 n_i \vec{a}_i$$

definitions of two BL's :  $n_i$   $m_j$  integer

$$\vec{K} \cdot \vec{R} = \sum_{i=1}^3 \sum_{j=1}^3 n_i m_j \underbrace{\vec{b}_j \cdot \vec{a}_i}_{2\pi \delta_{ij}} = 2\pi \sum_{i=1}^3 n_i m_i$$

some integer  $\equiv N$

$$\exp(i \vec{K} \cdot \vec{R}) = \exp(i 2\pi N) = 1$$

$$\vec{K} = \sum_{j=1}^3 m_j \vec{b}_j$$

$\cap$   
 $RL$

$$\vec{R} = \sum_{i=1}^3 n_i \vec{a}_i$$

$\cap$   
 $BL$

Theorem 2. Volume of the RL primitive cell

$$V_R = \frac{(2\pi)^3}{V}$$

where  $V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$  is the volume of the direct BL.

Proof: By vector algebra  $V_R = |\vec{B}_1 \cdot (\vec{B}_2 \times \vec{B}_3)|$ .  
 let's use  $\vec{B}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$   
 or  $\vec{B}_1 = \frac{2\pi}{V} (\vec{a}_2 \times \vec{a}_3)$ .

We have  $V_R = \frac{2\pi}{V} \left| \underbrace{(\vec{a}_2 \times \vec{a}_3)}_{\text{denote } \vec{A}} \cdot (\vec{B}_2 \times \vec{B}_3) \right|$

$$\vec{A} \cdot (\vec{B}_2 \times \vec{B}_3) = (\vec{A} \times \vec{B}_2) \cdot \vec{B}_3$$

$$\vec{A} \times \vec{B}_2 = (\vec{a}_2 \times \vec{a}_3) \times \vec{B}_2$$

vector  
algebra:

$$\begin{aligned}\vec{A} \times (\vec{B} \times \vec{C}) &= \vec{B} (\vec{A} \cdot \vec{C}) - \vec{C} (\vec{A} \cdot \vec{B}) \\ (\vec{A} \times \vec{B}) \times \vec{C} &= \vec{B} (\vec{A} \cdot \vec{C}) - \vec{A} (\vec{B} \cdot \vec{C})\end{aligned}$$

$$(\vec{a}_2 \times \vec{a}_3) \times \vec{B}_2 = \vec{a}_3 (\vec{a}_2 \cdot \vec{B}_2) - \vec{a}_2 (\vec{a}_3 \cdot \vec{B}_2)$$

We Know  $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \Rightarrow$

$$\underbrace{(\vec{a}_2 \times \vec{a}_3) \times \vec{b}_2}_{\vec{A}} = \vec{a}_3 (\underbrace{\vec{a}_2 \cdot \vec{b}_2}_{2\pi}) - \vec{a}_2 (\underbrace{\vec{a}_3 \cdot \vec{b}_2}_{\phi}) = 2\pi \vec{a}_3$$

Now  $V_R = \frac{2\pi}{v} \cdot |\vec{A} \cdot (\vec{b}_2 \times \vec{b}_3)| = \frac{2\pi}{v} \underbrace{|(\vec{A} \times \vec{b}_2) \cdot \vec{b}_3|}_{2\pi \vec{a}_3}$

*auxiliary vector*  $\vec{A} = \vec{a}_2 \times \vec{a}_3$

$$V_R = \frac{2\pi}{v} \cdot 2\pi \left| \underbrace{\vec{a}_3 \cdot \vec{b}_3}_{2\pi} \right| = \frac{(2\pi)^3}{v} \quad \checkmark$$

Theorem 3. The RL of the RL = <sup>original</sup> lattice

Proof: Consider  $\{\vec{b}_i\}$  as primitive vectors.

Construct RL :

$$\vec{c}_1 = \frac{2\pi}{v_R} (\vec{b}_2 \times \vec{b}_3) \quad \stackrel{2\pi}{\stackrel{\vec{a}_1}{\approx}} \quad \vec{c}_2 = \frac{2\pi}{v_R} \vec{b}_3 \times \vec{b}_1 \quad \stackrel{2\pi}{\stackrel{\vec{a}_2}{\approx}} \\ \vec{c}_3 = \frac{2\pi}{v_R} \vec{b}_1 \times \vec{b}_2 \quad \stackrel{2\pi}{\stackrel{\vec{a}_3}{\approx}}$$

where  $v_R = |\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)| = \frac{(2\pi)^3}{v} \quad (\text{Th.2})$

$$\text{Consider, e.g., } \vec{C}_1 : \quad \vec{B}_3 = \frac{2\pi}{v} \vec{a}_1 \times \vec{a}_2$$

$$\vec{C}_1 = \frac{2\pi}{v_R} \cdot \vec{B}_2 \times \frac{2\pi}{v} (\vec{a}_1 \times \vec{a}_2) \quad \leftarrow \text{ substitute}$$

$$\vec{C}_1 = \frac{(2\pi)^2}{v} \cdot \frac{1}{v_R} \vec{B}_2 \times (\vec{a}_1 \times \vec{a}_2)$$

$$\vec{C}_1 = \frac{(2\pi)^2}{v} \cdot \frac{1}{v_R} \cdot \left\{ \vec{a}_1 (\vec{B}_2 \cdot \vec{a}_2) - \vec{a}_2 (\vec{B}_2 \cdot \vec{a}_1) \right\}_{\frac{2\pi}{v}} \phi$$

$$\vec{C}_1 = \frac{(2\pi)^3}{v^3} \cdot \frac{1}{v_R} \vec{a}_1 = \vec{a}_1$$

Analogously  $\vec{C}_2 = \vec{a}_2$  and  $\vec{C}_3 = \vec{a}_3$

The RL of RL = original lattice

In Solid State Physics usually

direct BL is in real  $\vec{r}$ -space

reciprocal lattice is in "momentum"  $\vec{k}$ -space  
( $\vec{k}$ , wave number)

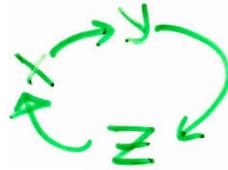
# Important examples

## ① Simple cubic BL

$$\vec{a}_1 = a \hat{x} \quad \vec{a}_2 = a \hat{y} \quad \vec{a}_3 = a \hat{z}$$

$$V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| = a^3$$

$$V_R = \frac{(2\pi)^3}{V} = \frac{(2\pi)^3}{a^3}$$



$$\vec{b}_1 = \frac{2\pi}{V} \quad \vec{a}_2 \times \vec{a}_3 = \frac{2\pi}{V} a^2 \quad \hat{y} \times \hat{z} = \frac{2\pi}{a} \hat{x}$$

$$\vec{b}_2 = \frac{2\pi}{V} \quad \vec{a}_3 \times \vec{a}_1 = \frac{2\pi}{V} a^2 \quad \hat{z} \times \hat{x} = \frac{2\pi}{a} \hat{y}$$

$$\vec{b}_3 = \frac{2\pi}{V} \quad \vec{a}_1 \times \vec{a}_2 = \frac{2\pi}{V} a^2 \quad \hat{x} \times \hat{y} = \frac{2\pi}{a} \hat{z}$$

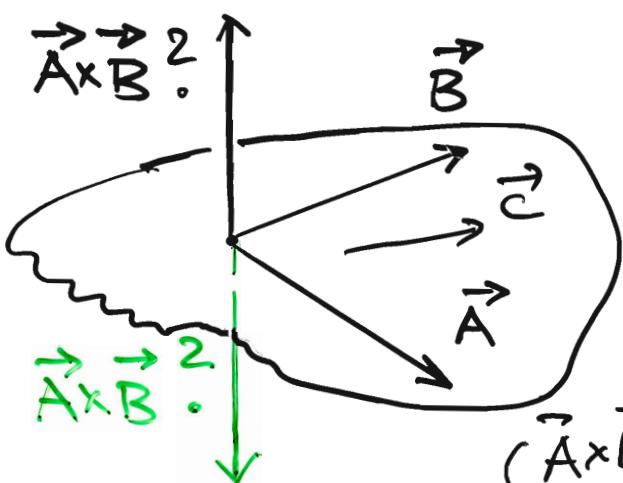
Simple Cubic  
with lattice  
constant  $a$

$$V = a^3$$

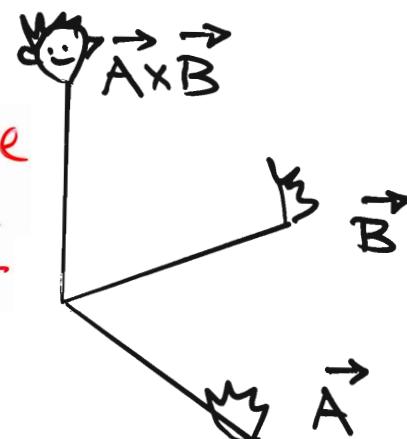
Reciprocal :  
simple cubic  
with latt. const.  $\frac{2\pi}{a}$

$$V_R = \left(\frac{2\pi}{a}\right)^3 = \frac{(2\pi)^3}{V}$$

Direction of  $\vec{A} \times \vec{B}$  ?



The rule  
of the  
RIGHT  
leg :



## III. Face-centered cubic BL (FCC) $\vartheta = \frac{a^3}{4}$

$$\vec{a}_1 = \frac{1}{2}a(\hat{x} + \hat{y}) \quad \vec{a}_2 = \frac{1}{2}a(\hat{x} + \hat{z}) \quad \vec{a}_3 = \frac{1}{2}(\hat{y} + \hat{z})$$

RL:  $\vec{B}_1 = \frac{2\pi}{v} \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{v} \cdot \frac{a^2}{4} \cdot (\hat{x} + \hat{z}) \times (\hat{y} + \hat{z})$

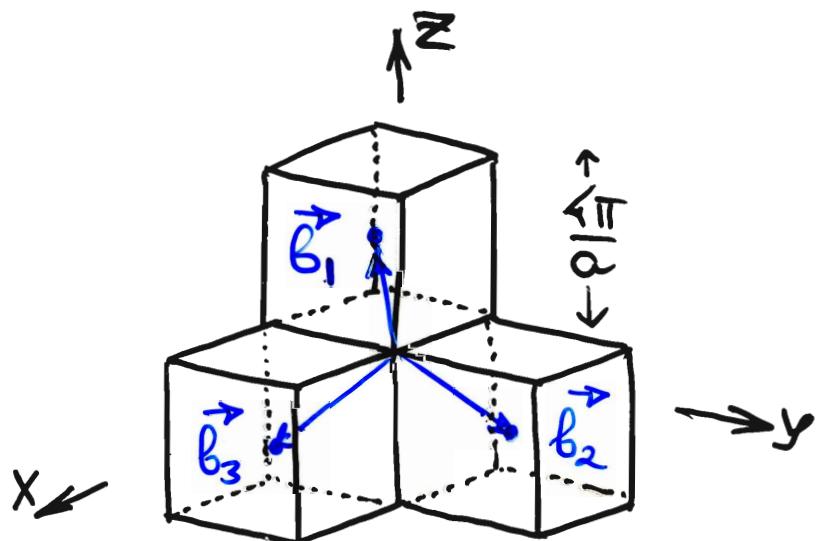
$\checkmark \quad \vec{B}_1 = \frac{2\pi}{a} (\hat{z} - \hat{y} - \hat{x}) = \frac{4\pi}{a} \cdot \frac{1}{2} (-\hat{x} - \hat{y} + \hat{z})$

$$\vec{B}_2 = \frac{2\pi}{v} \vec{a}_3 \times \vec{a}_1 = \frac{2\pi}{v} \cdot \frac{a^2}{4} \cdot (\hat{y} + \hat{z}) \times (\hat{x} + \hat{y})$$

$\checkmark \quad \vec{B}_2 = \frac{2\pi}{a} (-\hat{z} + \hat{y} - \hat{x}) = \frac{4\pi}{a} \cdot \frac{1}{2} (-\hat{x} + \hat{y} - \hat{z})$

$$\vec{B}_3 = \frac{2\pi}{v} \vec{a}_1 \times \vec{a}_2 = \frac{2\pi}{v} \cdot \frac{a^2}{4} \cdot (\hat{x} + \hat{y}) \times (\hat{x} + \hat{z})$$

$\checkmark \quad \vec{B}_3 = \frac{2\pi}{a} (-\hat{y} - \hat{z} + \hat{x}) = \frac{4\pi}{a} \cdot \frac{1}{2} (\hat{x} - \hat{y} - \hat{z})$



BCC primitive vectors!

BL

RL

$$\text{SC } (a) \rightarrow \text{SC } \left(\frac{2\pi}{a}\right)$$

$$\text{FCC } (a) \rightarrow \text{BCC } \left(\frac{4\pi}{a}\right)$$

$$\text{BCC } (a) \rightarrow \text{FCC } \left(\frac{4\pi}{a}\right)$$

Simple hexagonal  $(a, c)$   $\rightarrow$  Simple hexagonal  $\left(\frac{4\pi}{\sqrt{3}a}, \frac{2\pi}{c}\right)$

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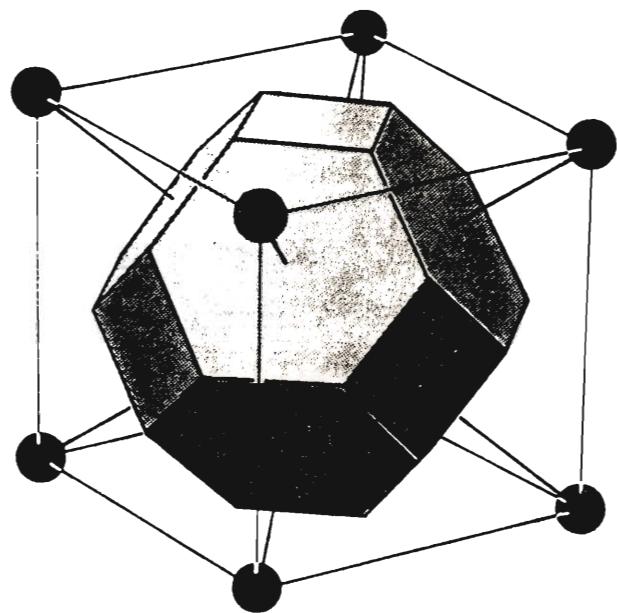
### First Brillouin Zone

is the Wigner-Seitz cell  
of the reciprocal lattice

Direct lattice :  $\vec{r}$ -space (coordinates)

Reciprocal lattice :  $\vec{k}$ -space (wave vectors)

First Brillouin Zone is just  
some region in  $\vec{k}$ -space

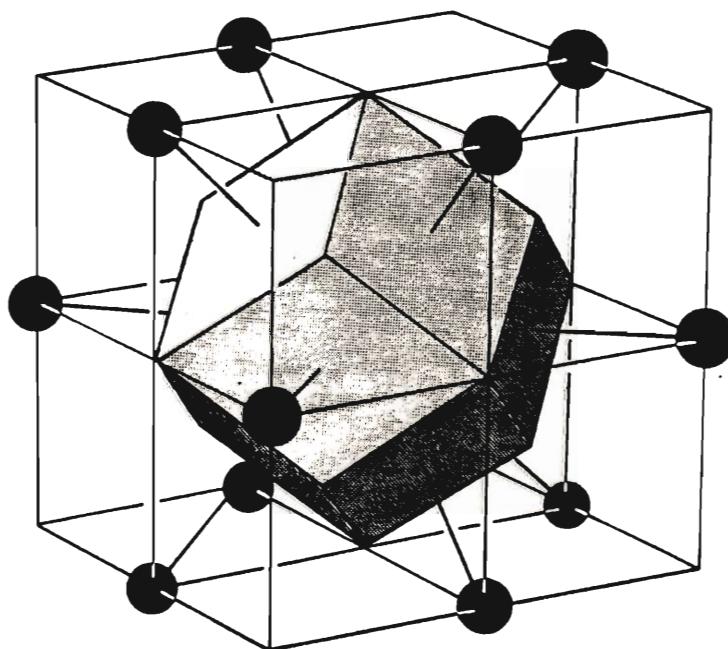


truncated octahedron  
(hexagons + squares)

Wigner-Seitz cell  
for BCC ( $\vec{k}$ -space)  
lattice const.  $a$

First Brillouin  
Zone for FCC  
( $\vec{k}$ -space)

$$\frac{4\pi}{a}$$



rhombic dodecahedron

Wigner-Seitz cell  
for FCC ( $\vec{k}$ -space)  
lattice const.  $a$

First Brillouin  
Zone for BCC  
( $\vec{k}$ -space)

$$\frac{4\pi}{a}$$