

Reciprocal Lattice

- Start with Bravais lattice $\{\vec{R}\}$. $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$.
- The reciprocal lattice is all vectors \vec{K} satisfying $e^{i\vec{K} \cdot \vec{R}} = 1$, for all \vec{R} ,
~~True if and only if~~ $\vec{K} \cdot \vec{a}_i = 2\pi M_i$ \checkmark integer.
- The reciprocal lattice is closed under addition & subtraction.
 e.g. \vec{K}_1 and \vec{K}_2 are RLV's, then so is $\vec{K} = \vec{K}_1 + \vec{K}_2$
 $e^{i\vec{K} \cdot \vec{R}} = e^{i\vec{K}_1 \cdot \vec{R}} e^{i\vec{K}_2 \cdot \vec{R}} = 1$.
- ~~Will show in HW~~
- This implies the reciprocal lattice is itself a Bravais lattice
 — see A&M Problem 4.8.

• Primitive RL vectors:

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

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

$\Rightarrow \vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \Rightarrow \vec{b}_i$'s are RLV's.

- Want to show that \vec{b}_i are also primitive vectors for RL:

• \vec{b}_i are linearly independent, so for any vector \vec{k} ,

$$\vec{k} = x_1 \vec{b}_1 + x_2 \vec{b}_2 + x_3 \vec{b}_3 \quad (x_i \text{ not necessarily integers})$$

• \vec{k} is a RLV if and only if $\vec{k} \cdot \vec{R} = 2\pi \times \text{integer}$
for all \vec{R}

$$\Leftrightarrow 2\pi(x_1 n_1 + x_2 n_2 + x_3 n_3) = 2\pi \times \text{integer for } \underline{\text{all integers }} n_1, n_2, n_3$$

\rightarrow Can only be true if x_i are integers

\Rightarrow All RLV's are integer linear combinations
of the \vec{b}_i . ✓

- Volume of RL primitive cell is $V_R = |\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)| = \frac{(2a)^3}{V_K}$
 volume
of original
primitive cell

- Wigner-Seitz cell of RL is called "First Brillouin Zone"
- Reciprocal of the reciprocal lattice is the original lattice we started with.

d=2 RL primitive vectors

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \hat{\vec{z}}}{|\vec{a}_1 \times \vec{a}_2|} ; \quad \vec{b}_2 = 2\pi \frac{\hat{\vec{z}} \times \vec{a}_1}{|\vec{a}_1 \times \vec{a}_2|}$$

- Examples: (1) Square is its own RL: $\vec{a}_1 = a\hat{x} ; \vec{a}_2 = a\hat{y}$
 $\vec{b}_1 = \frac{2\pi}{a}\hat{x} ; \vec{b}_2 = \frac{2\pi}{a}\hat{y}$.

(2) Simple cubic lattice is its own RL

(3) FCC RL of BCC is FCC (and vice-versa)

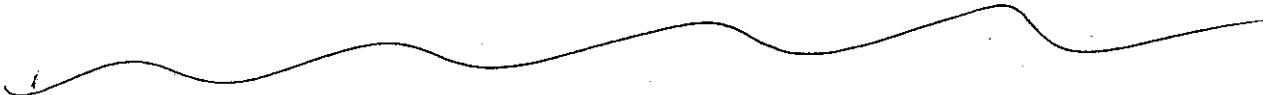
- Suppose we have a function $f(\vec{r})$ periodic in the original Bravais lattice, $f(\vec{r}) = f(\vec{r} + \vec{R})$ for all \vec{R} . Then the Fourier decomposition is:

$$f(\vec{r}) = \sum_{\vec{K}} e^{i\vec{K} \cdot \vec{r}} \tilde{f}(\vec{K})$$

\hookrightarrow in RL

- The RL is the set of allowed Fourier components of a function periodic in the original Bravais lattice.

→ This is why it showed up in our scattering experiment!



NB: No such thing as RL of lattice with basis. In such cases we use the RL of the underlying Bravais lattice (e.g. FCC for diamond structure).
 \Rightarrow BCC RL).

"Geometrical Interpretation" of RL

- RLV's are normal vectors to lattice planes in the original Bravais lattice.
- Suppose we have a lattice plane with unit normal \hat{n} , and spacing d between adjacent planes. Then $\vec{K} = \frac{2\pi}{d}\hat{n}$ is an RLV.
- Conversely, if \vec{K}_0 is the shortest RLV parallel to some RLV \vec{K} , then $\vec{K}_0 = \frac{2\pi}{d}\hat{n}$, where \hat{n} and d are as above for some set of lattice planes.

(This is proved in A&M Ch.5)

Lattice Directions (Notation)

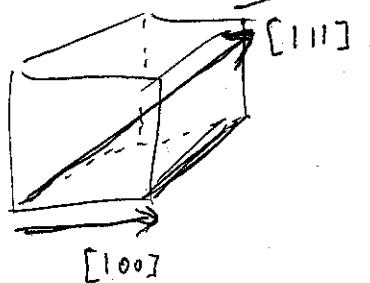
- Suppose we have Bravais lattice with $\vec{a}_1, \vec{a}_2, \vec{a}_3$ and its RL with $\vec{b}_1, \vec{b}_2, \vec{b}_3$.

These integers should have no common factor.

$$[n_1 n_2 n_3] \leftrightarrow n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

direction

e.g. (simple cubic)



[111] direction

is written [100].

$\langle n_1 n_2 n_3 \rangle$ → all directions related by symmetry to $[n_1 n_2 n_3]$

(simple cubic)

e.g. $\langle 100 \rangle$ includes [100], [010], [T00], etc.

(hkl) direction $\leftrightarrow h \vec{b}_1 + k \vec{b}_2 + l \vec{b}_3$ (normal to set of lattice planes)

{hkl} \leftrightarrow all directions (hkl) related by symmetry.

(7)

NB: These notations depend on arbitrary choice of primitive vectors. For cubic crystals (including FCC, BCC), a ~~the~~ simple cubic Bravais lattice is used so that

$$\vec{a}_1 = a \hat{x}, \vec{b}_1 = \frac{2\pi}{a} \hat{x}, \text{ etc.}$$