Reciprocal Space

Motivation:

- interested in physical phenomena in crystals
  - → often involve waves (e^- waves, vibrations, electromagnetic waves)

Space of waves is recirprocal space

plane wave: $e^{i\vec{k}\vec{r}}$ with wave vector $\vec{k} = \frac{2\pi}{\lambda}$

→ convenient to think of crystal structures in reciprocal space

Literature: Kittel, Chap 2

in 1D

direct lattice $R_n = \vec{a}n$

reciprocal lattice $G_m = \left(\frac{2\pi}{\vec{a}}\right)m$

$\vec{k} \to \vec{k} + G_m$ reproduces same wave!

$$e^{ikR_n} \to e^{i(k+G_m)R_n} \to e^{ikR_n}\, e^{iG_m R_n} \to e^{ikR_n}\, \underbrace{e^{i\left(\frac{2\pi}{a}m\right)an}}_{1}$$

<u>in any dimension</u>

define reciprocal lattice as points $\vec{G}$ such that

$e^{i\vec{G}\vec{R}_n} = 1$ for all $\vec{R}_n$ in direct lattice

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

"guess" the reciprocal lattice vectors $\vec{b}_i$

$$\vec{b}_i \cdot \vec{a}_j = 2\pi\,\delta_{ij}$$

with

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

for $i,j,k = 1,2,3$

2 3 1

3 1 2

$$\vec{b}_1\cdot\vec{a}_1 = \left(2\pi \frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}\right)\cdot a_1 = 2\pi$$

$$\vec{b}_1\cdot\vec{a}_2 = \left(\;\sim\;\right)\cdot a_2 = 0$$

$\vec{b}_i$ = primitive reciprocal lattice vectors (PRLVs)

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

Proof that this defines a lattice

$$e^{iG\cdot R} = e^{i(m_1 b_1 + m_2 b_2 + m_3 b_3)(n_1 a_1 + n_2 a_2 + n_3 a_3)}$$

$$= e^{i 2\pi (m_1 n_1 + m_2 n_2 + m_3 n_3)} = 1$$

$\rightarrow$ only for $n, m \in \mathbb{Z}$

facts:

- reciprocal lattice is Fourier transform of real lattice
- in 2D, same rules apply
- reciprocal lattice of fcc is bcc and vice versa