Lecture 8
Waves in and into/out-of Crystal

Crystal Translation Symmetry and
Bloch's theorem

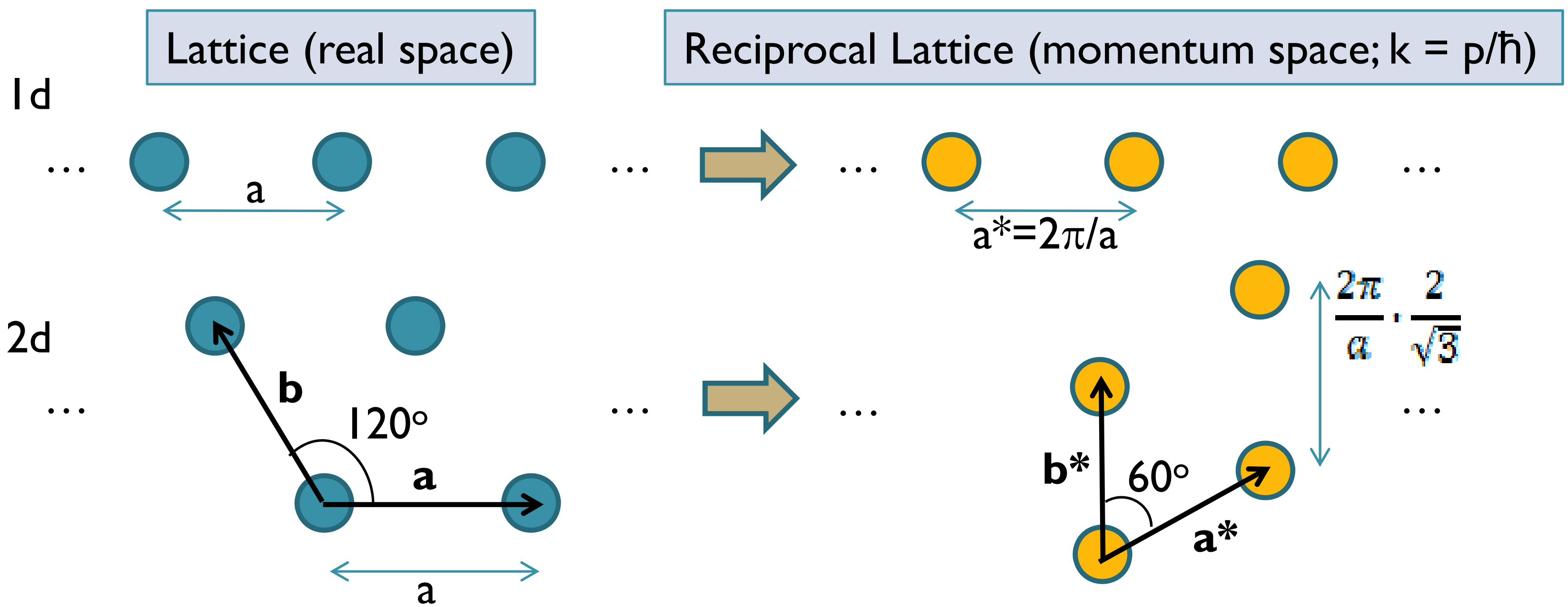
FF ch. 11 – Reciprocal Lattice

- Given the lattice of **a, b, c,** (in 3d; 2d, 1d analogous)

  <u>define reciprocal lattice</u> **a*,b*,c***:

  $$\mathbf{a}^*\cdot\mathbf{b} = \mathbf{a}^*\cdot\mathbf{c} = \mathbf{b}^*\cdot\mathbf{c} = \mathbf{b}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{b} = 0$$

  $$\mathbf{a}^*\cdot\mathbf{a} = \mathbf{b}^*\cdot\mathbf{b} = \mathbf{c}^*\cdot\mathbf{c} = 2\pi$$ (and keep handed-ness)



Reminder

Reciprocal Lattice

$\mathbf{a}^*=2\pi(\mathbf{b}\times\mathbf{c})/V$

$\mathbf{b}^*=2\pi(\mathbf{c}\times\mathbf{a})/V$

$\mathbf{c}^*=2\pi(\mathbf{a}\times\mathbf{b})/V$

Volume of unit cell in real space

$V = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$

Volume of unit cell in reciprocal space

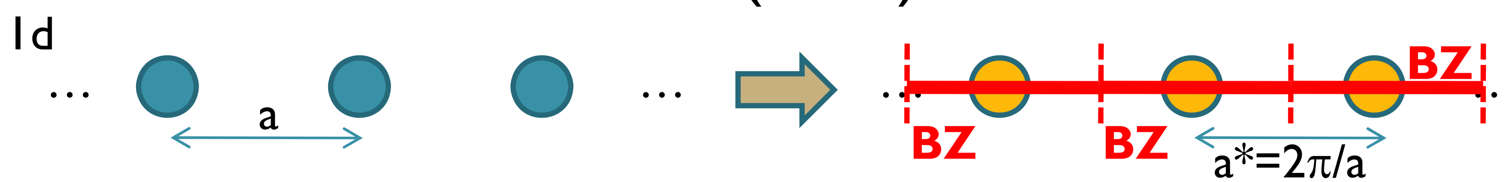
$V^* = \mathbf{a}^*\cdot(\mathbf{b}^*\times\mathbf{c}^*) = (2\pi)^3/V$

(Basis of Wilson's rule for general lattice)

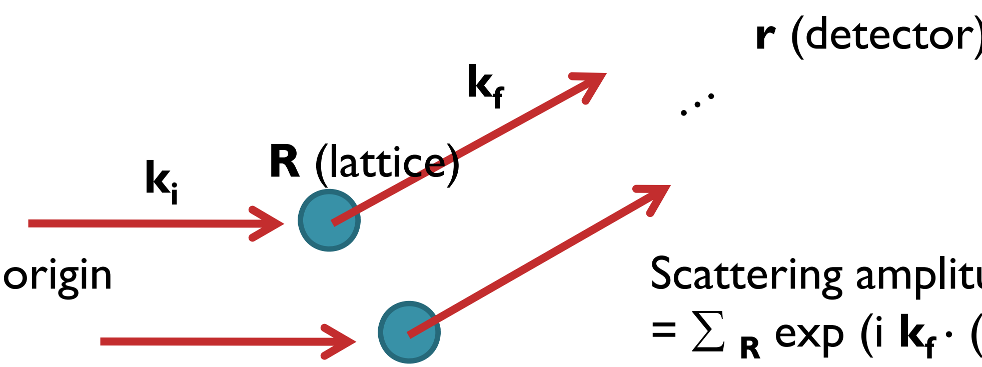
H&H, 11.2.2

FF ch. 11 – Reciprocal Lattice

- WS cell of R.L.– (first) **Brillouin zone**



- LOTS of Physics, e.g. Bragg's law



light source at origin

Bragg's law: $\mathbf{q} = \mathbf{G}$
$\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$
$\mathbf{G} = m\,\mathbf{a}^* + n\,\mathbf{b}^* + o\,\mathbf{c}^*$
(m,n,o = integer)

$f \propto$ atomic and structural scattering form factors and spherical wave attenuation factor (1/distance)

Scattering amplitude
$= \sum_{\mathbf{R}} \exp(i\,\mathbf{k}_f \cdot (\mathbf{r} - \mathbf{R}))\,\exp(i\,\mathbf{k}_i \cdot \mathbf{R})\,f(\mathbf{q})$
$\propto \sum_{\mathbf{R}} \exp(-i\,\mathbf{q} \cdot \mathbf{R})$
= <u>N if **q** is a R.L. vector, 0 otherwise</u>
(N = total number of lattice points)

Miller index is (m,n,o) for **G** normal to the plane

Reminder

Structural Factor

X-Ray Scattering Amplitude is given by

$$\sum_{\mathbf{R}} \exp(i\, \mathbf{q} \cdot \mathbf{R}) \sum_{j} f_j(\mathbf{q}) \exp(i\, \mathbf{q} \cdot \mathbf{r}_j)$$

(j = index running over atoms in the basis)

The 2nd summation is called a structural factor (S_G) and $f_j(q)$ is an atomic form factor

$$S_G = \sum_{j} f_j(\mathbf{q}) \exp(i\, \mathbf{q} \cdot \mathbf{r}_j)$$

H&H 11.2.1

Crystal Momentum Conservation

- $\mathbf{k_f} - \mathbf{k_i} = \mathbf{G}$ for Bragg Scattering
- This can be generalized for inelastic processes to (Bloch's theorem)

  $$\mathbf{k_f} - \mathbf{k_i} - \mathbf{q_e} = \mathbf{G}$$

  which holds for inelastic scattering for all experiments involving waves (electron, neutron, photon …) or any scattering processes that occur inside the crystal.
- Combining with the energy conservation rule, dispersion relations of phonons, electrons, spin waves etc. are routinely measured by neutron, photon, electrons as probes.

H&H 11,12