Lecture 3

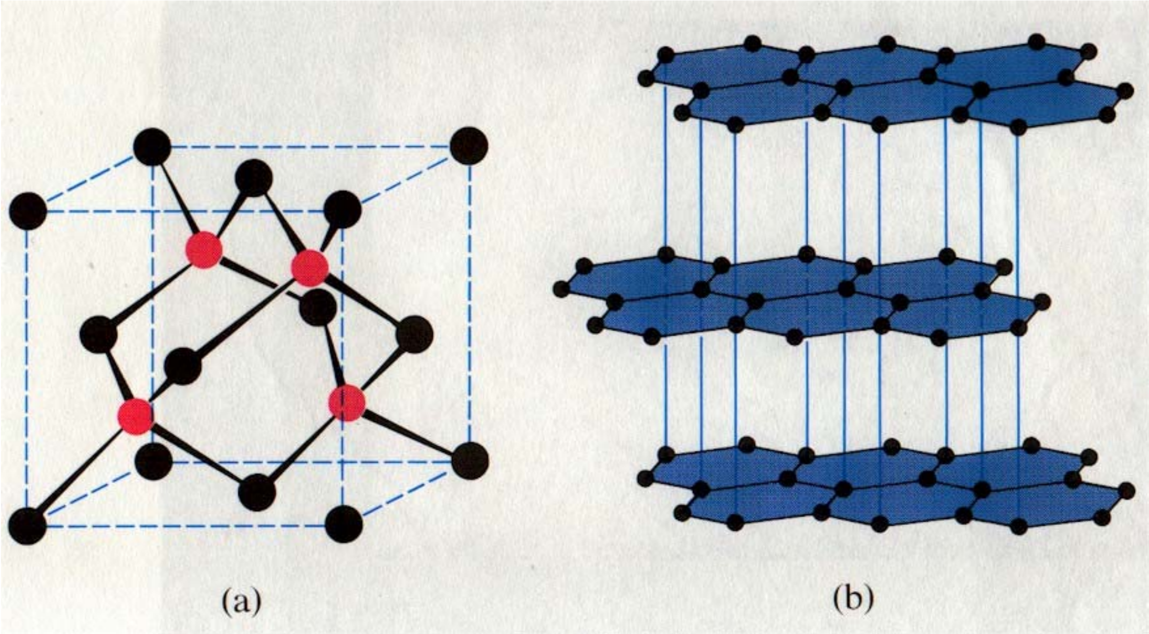
Waves in Crystal

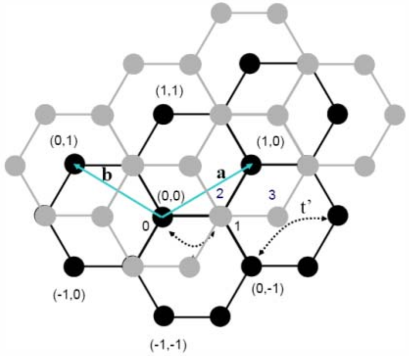
Crystal is nature's diffraction grating
for any wave, i.e. for any particle!

Interjection just due to the homework relevance

Crystal Bonding – Covalent Bonding

- Diamond
- Graphite





Top view
Gray=top
Black=next layer

http://library.tedankara.k12.tr/chemistry/vol2/allotropy/h76.jpg

fcc with two atom basis
000 and ¼, ¼, ¼
ZnS, Si, Ge, GaAs
sp3 covalent bonding

Hexagonal with four atom basis
sp2 bonding
Weak inter-plane bonding ("Van der Waals")
More stable than diamond!

How do we “See” the crystal?

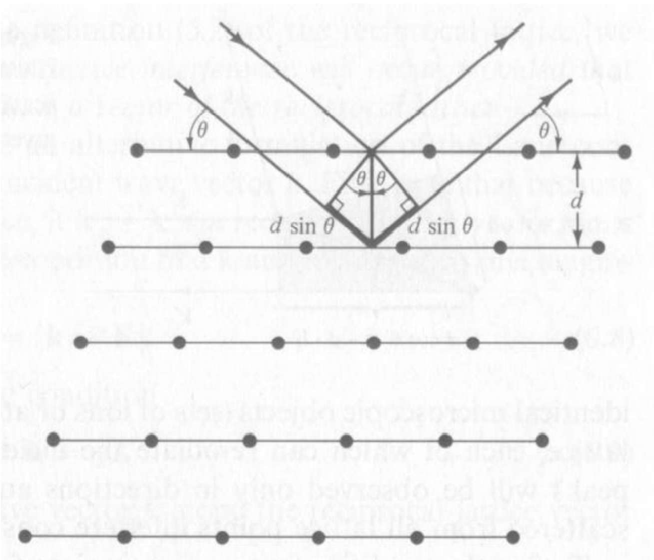
We need light with wavelength smaller than the length scale of the crystal.

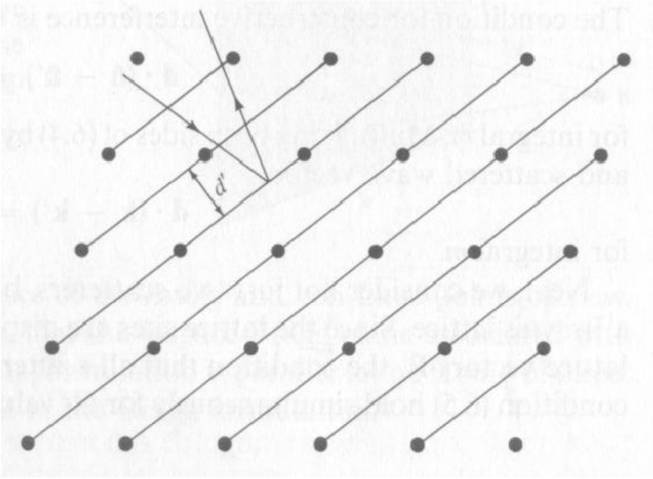
Typical crystal length scale is Å.

X-ray (~ 10 keV: “hard” X-ray)
Electron (~ 100 eV: “low energy” electron)
Neutron (~ 10-100 meV: “cold” or thermal)

Bragg Diffraction

$2d \sin \theta = n \lambda$





Reciprocal Lattice

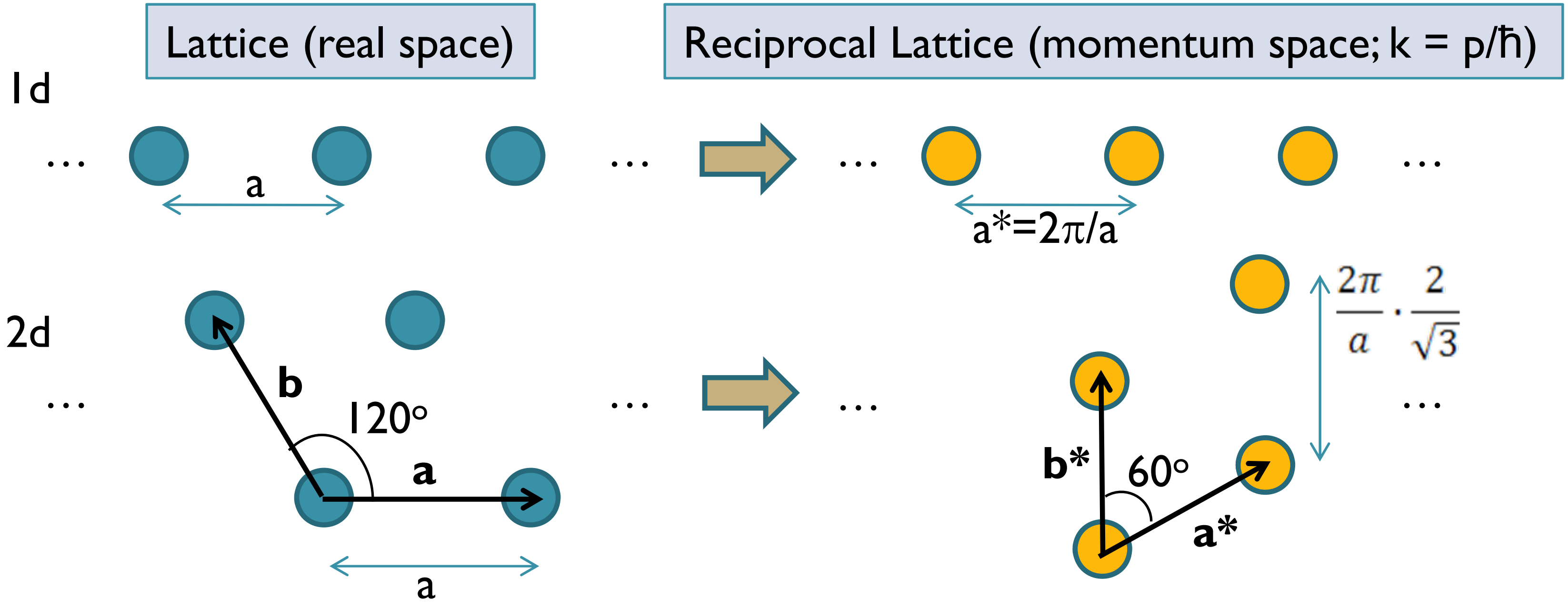
- Given the lattice of **a, b, c,** (in 3d; 2d, 1d analogous)

  <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)



Lattice (real space)

Reciprocal Lattice (momentum space; k = p/ħ)

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

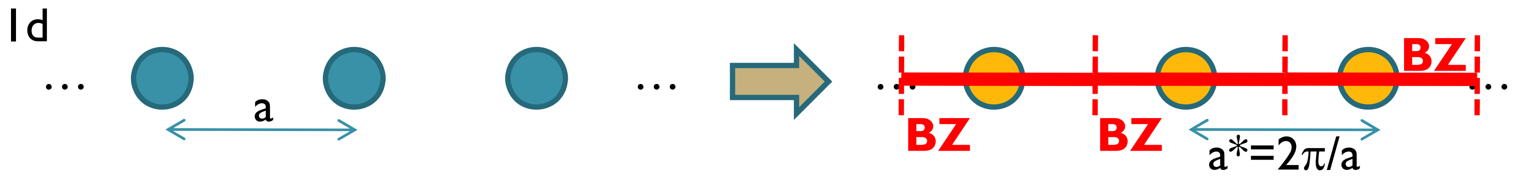
$V^* = \mathbf{a}^* \cdot (\mathbf{b}^* \times \mathbf{c}^*) = (2\pi)^3/V$

(Basis of Wilson's rule for general lattice)

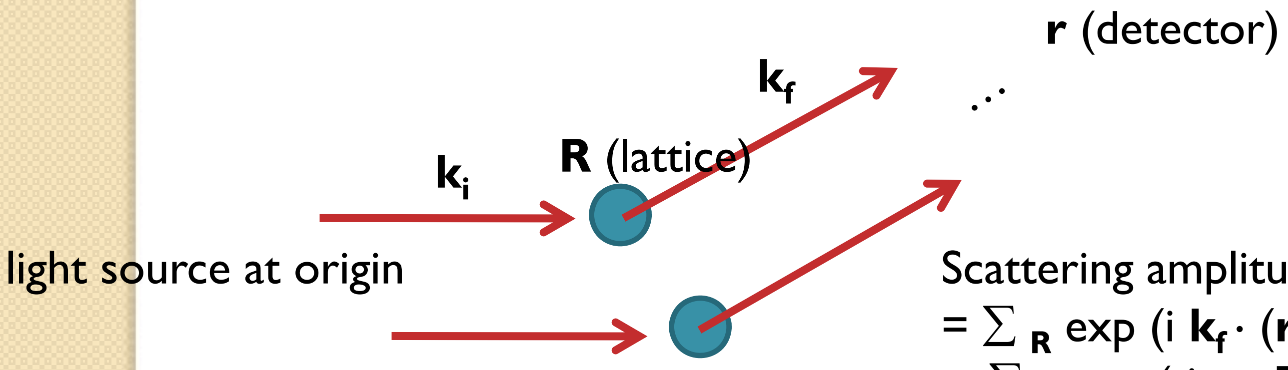
H&H, 11.2.2

Reciprocal Lattice

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



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



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

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)

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

$\sum_{\mathbf{R}} \exp(-i\, \mathbf{q} \cdot \mathbf{R})$

- = N [number of lattice points in the whole crystal] if q = 0 or a RL vector

  $\mathbf{q} = l\, \mathbf{a}^* + m\, \mathbf{b}^* + n\, \mathbf{c}^*$ (l,m,n = int)

  $\mathbf{R} = u\, \mathbf{a} + v\, \mathbf{b} + w\, \mathbf{c}$ (u,v,w = int)

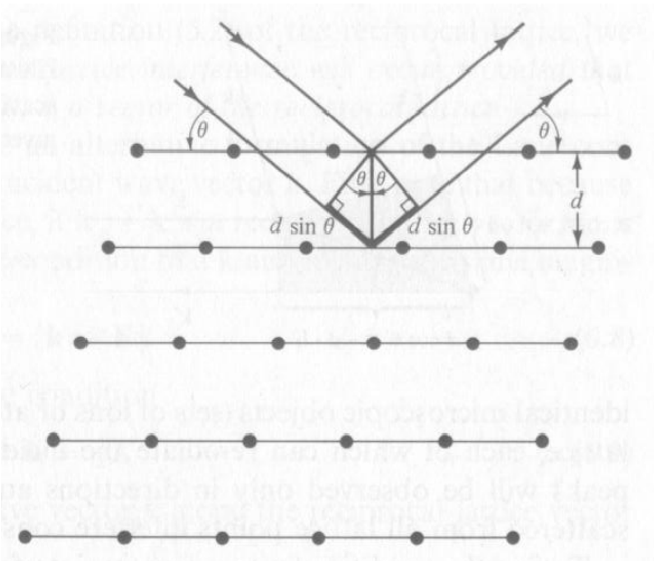
  $\mathbf{q} \cdot \mathbf{R} = 2\pi \times \text{integer}$
- = 0 [or O(1) which is 0 compared to N], otherwise, because phases are non-zero and equally distributed to make summands to cancel each other

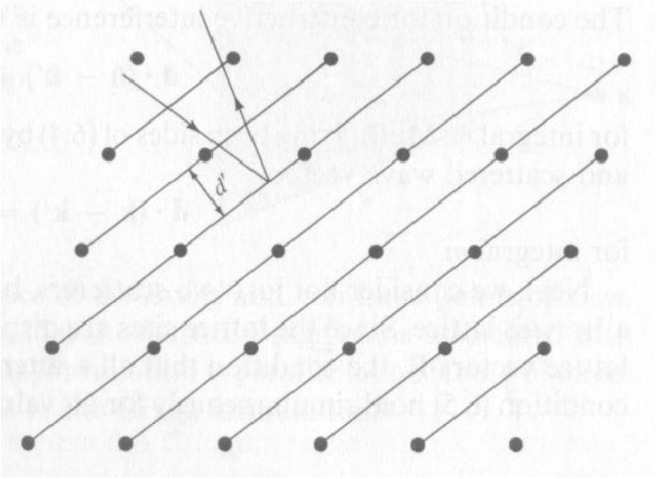
  [e.g. think 1D, with $\mathbf{q} = 0.5\mathbf{a}^*$]

  (will show more rigorously next class)

Bragg Diffraction

$$2d \sin\theta = n\lambda \qquad \Leftrightarrow \qquad \mathbf{q} = \mathbf{G}$$

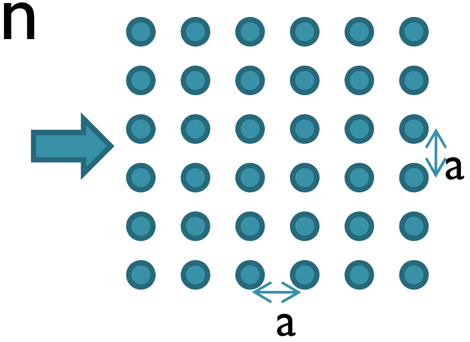




Question

Sections 1.4.1,2, of H&H

Consider Bragg Diffraction. Explain what may actually occur



(1) for a single value of λ (monochromatic light)

(2) for all λ values available in the beam (**Laue method**)

(3) for all θ values available at the same time (imagine a collection of crystallites with different orientation)

with but for monochromatic light (**powder method**)