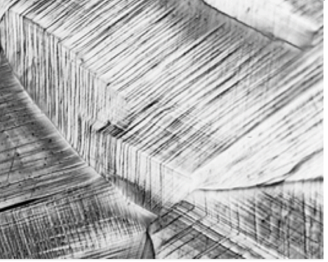
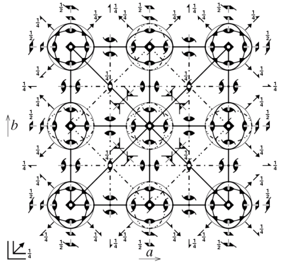
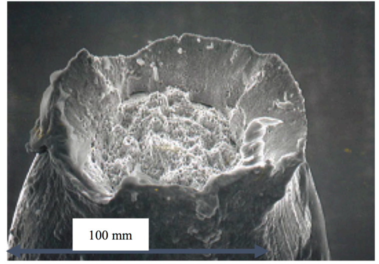
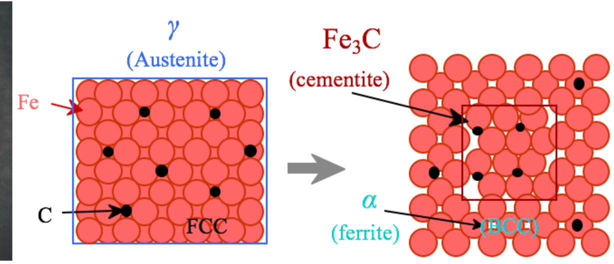








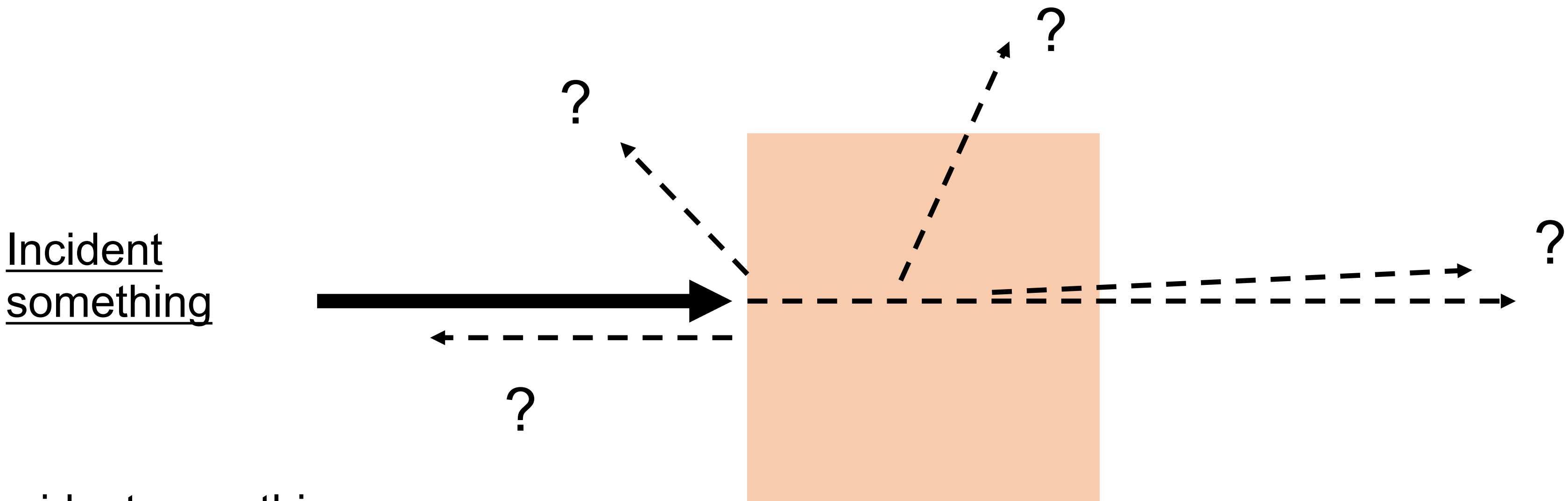
MEAM/MSE 507 Fundamentals of Materials

Prof. Jordan R. Raney

Week 5, Lecture 3: Introduction to diffraction

Asynchronous

Measuring material structure



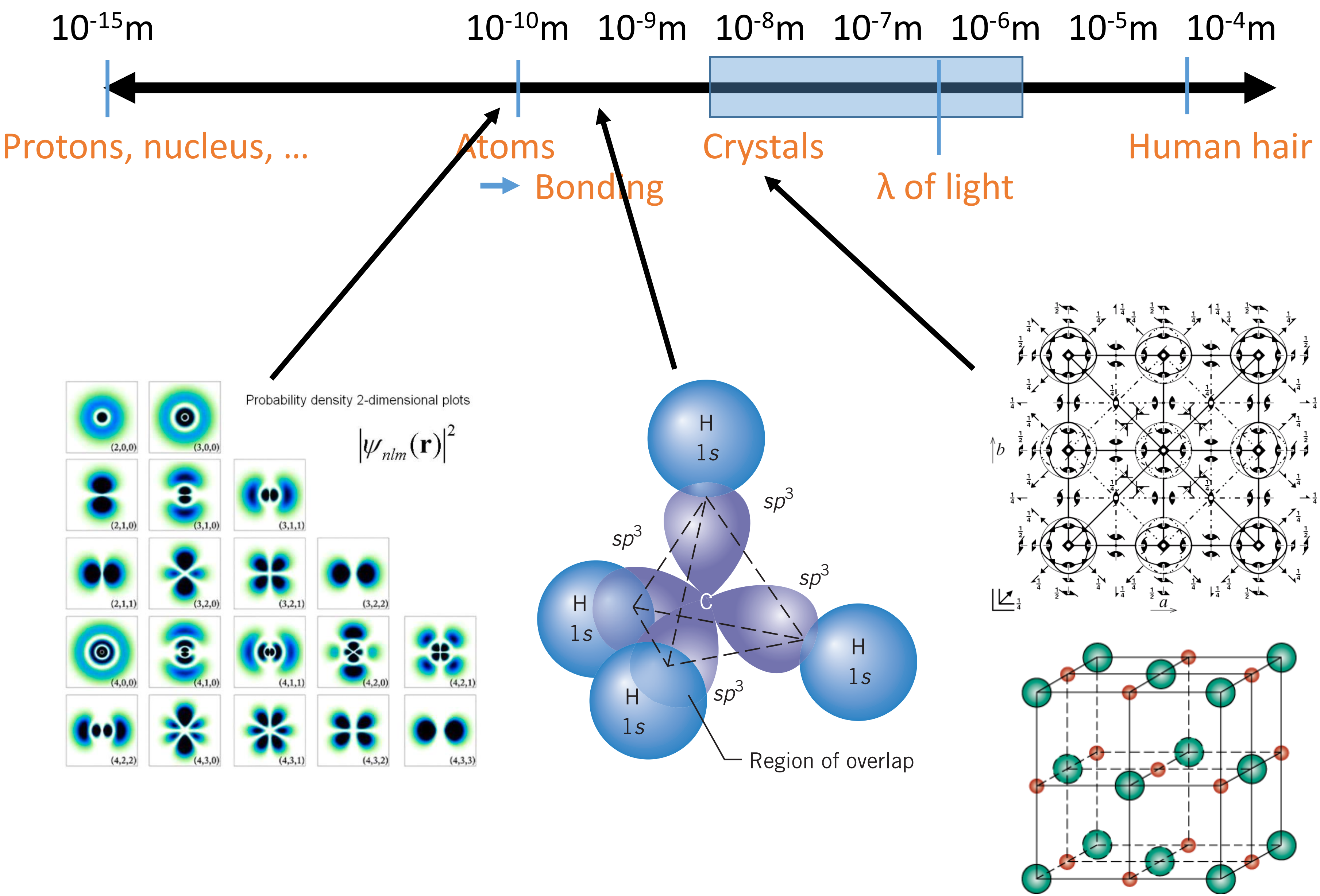
Incident something

- Need λ to be approximately the size of the structural features we are trying to see
- **X-rays**: cause electrons to oscillate and re-radiate
- **Electrons**: scattered by Coulomb interactions with positive atomic core
- **Neutrons**: scattered by nuclei (or unpaired electron spins)
- **γ-rays**: resonantly excite a nucleus, which later re-radiates

Scattered something

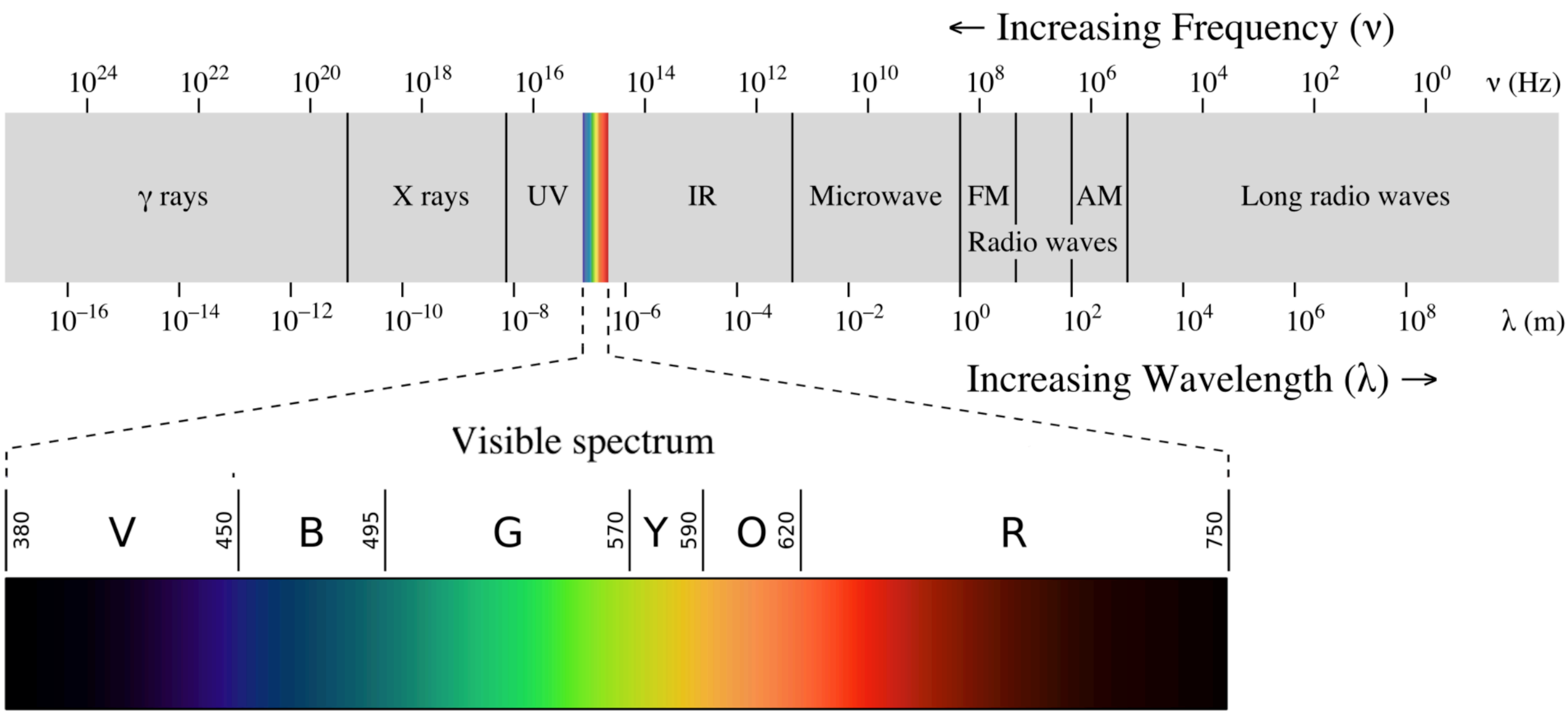
- Is the **phase information maintained**? If yes, this is **coherent** scattering. If no, this is **incoherent** scattering.
- Do the scattered “particles” have the same energy as the incident “particles”? If yes, **elastic** scattering. If no, **inelastic** scattering.
- **Diffraction** is associated with **coherent** and **elastic** scattering

Where we are



10^-15 m
10^-10 m
10^-9 m
10^-8 m
10^-7 m
10^-6 m
10^-5 m
10^-4 m
Protons, nucleus, …
Atoms
→ Bonding
Crystals
λ of light
Human hair
Probability density 2-dimensional plots
$|\psi_{nlm}(\mathbf{r})|^2$
(2,0,0)
(3,0,0)
(2,1,0)
(3,1,0)
(3,1,1)
(2,1,1)
(3,2,0)
(3,2,1)
(3,2,2)
(4,0,0)
(4,1,0)
(4,1,1)
(4,2,0)
(4,2,1)
(4,2,2)
(4,3,0)
(4,3,1)
(4,3,2)
(4,3,3)
H 1s
H 1s
H 1s
H 1s
C
sp^3
sp^3
sp^3
sp^3
Region of overlap
b
a

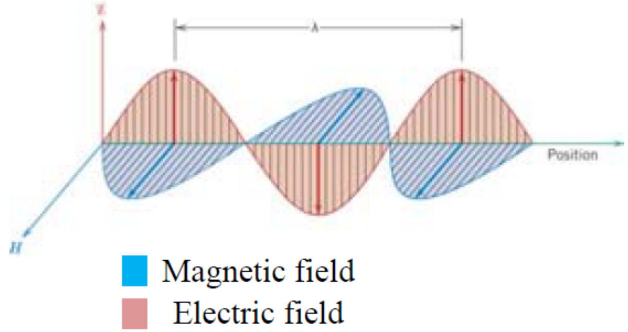
Electromagnetic radiation



Wikipedia

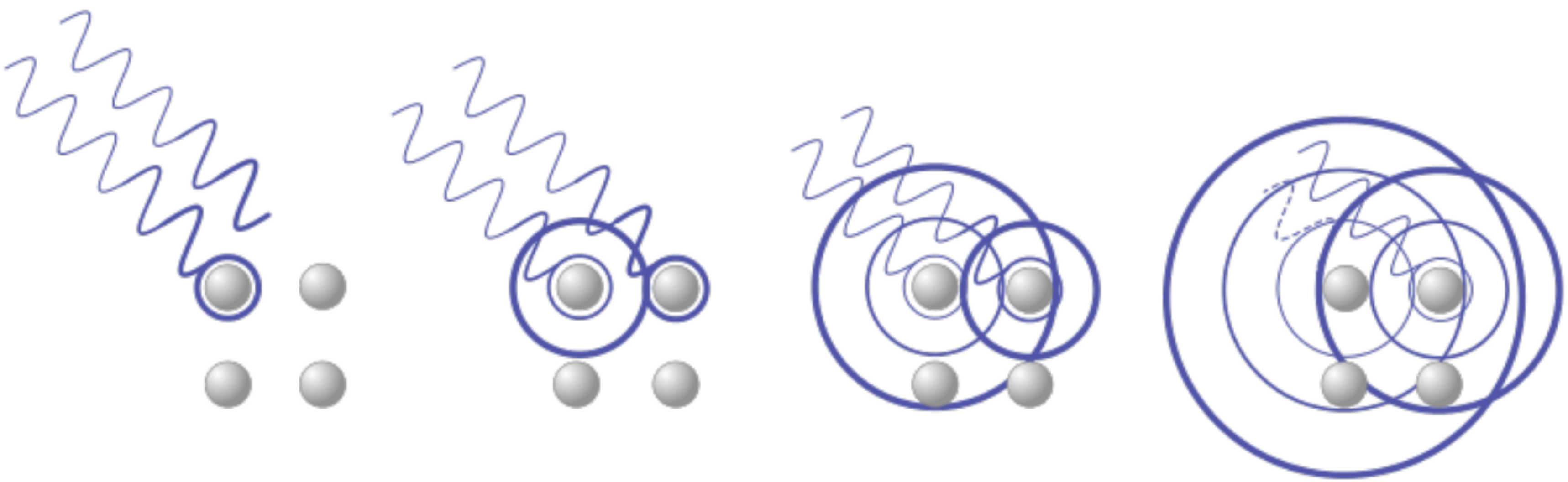
Scattering by atoms

- Beam passes by an atom, the EM waves interact with the electrons, can cause vibration, re-radiation, etc.



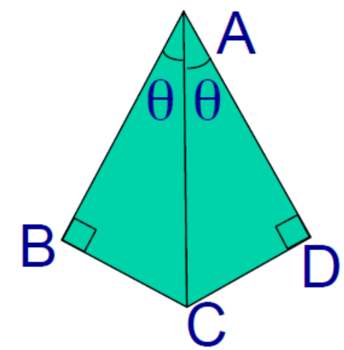
e$^-$ interact with both electric and magnetic fields → interact with light

- Superposition of waves scattered by atoms produces diffraction

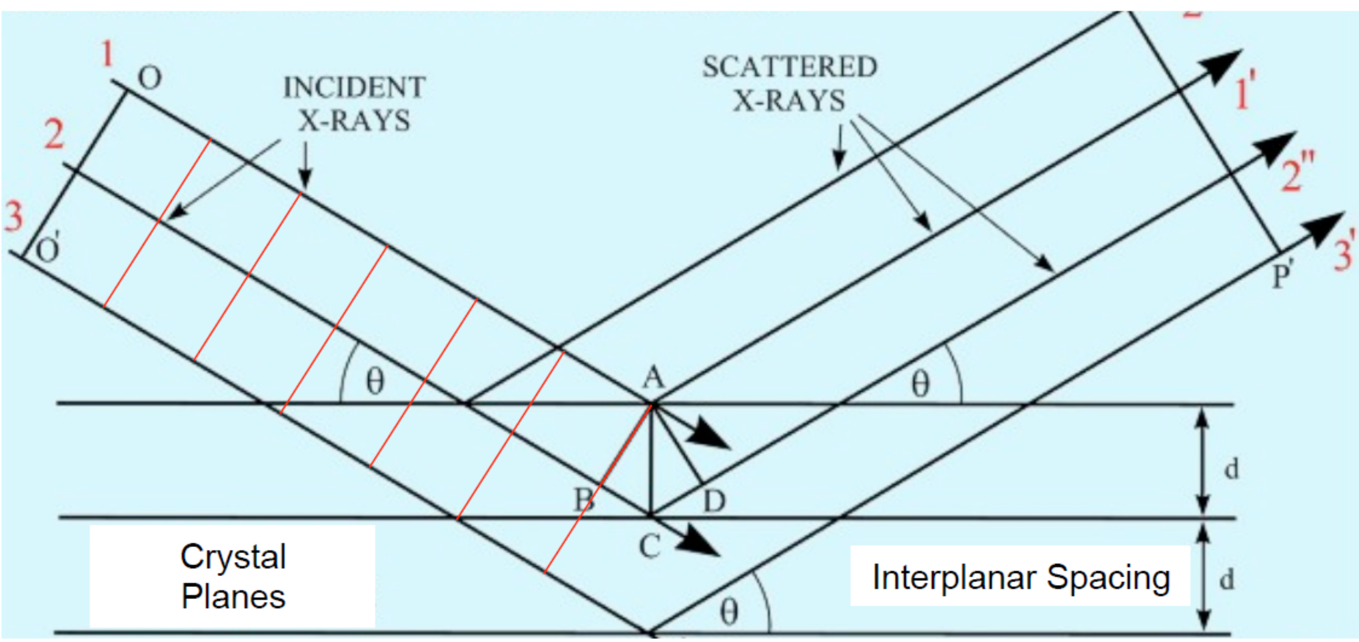


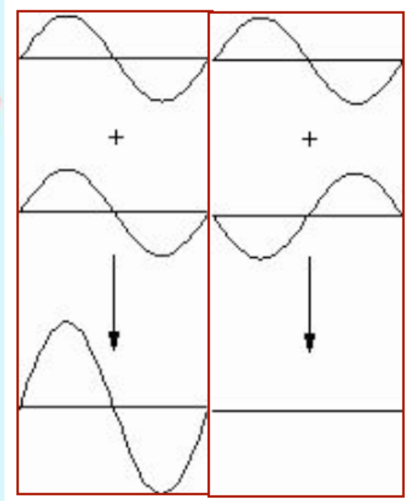
Coherent scattering by crystal planes

- Some of the incident wave scatters/reflects from the 1st atomic plane, some from 2nd, ….
- Angle of incidence = Angle of reflection, θ
- Wave from 2nd plane travels BC+CD further than 1st
- If BC+CD is $n\lambda$, constructive interference



Bragg's Law $$n\lambda = 2d\sin\theta$$





Interplanar spacings

- Spacing between atomic planes depends on which planes and which crystal structure
- Miller indices (hkl), unit cell dimensions a,b,c

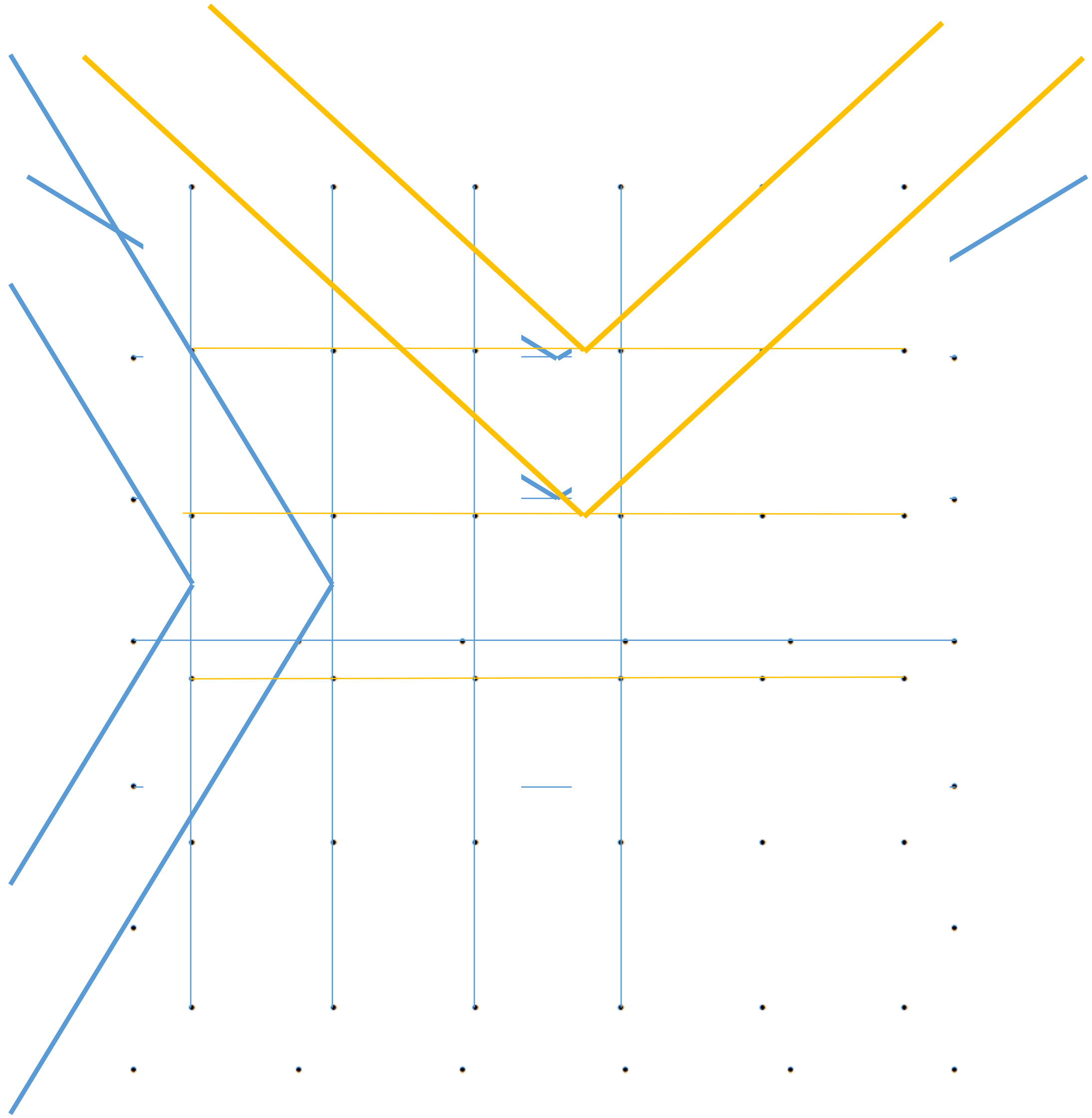
Cubic	Tetragonal	Orthorhombic	Hexagonal
$\frac{1}{d_{hkl}^2} = \frac{h^2+k^2+l^2}{a^2}$	$\frac{1}{d_{hkl}^2} = \frac{h^2+k^2}{a^2} + \frac{l^2}{c^2}$	$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$	$\frac{1}{d_{hkl}^2} = \frac{4}{3}\left(\frac{h^2+hk+k^2}{a^2}\right) + \frac{l^2}{c^2}$

- For other crystal structures – more complex
- **Example:** (111) planes in FCC Ni (a=3.52 Å), λ=2 Å

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{3.52\text{Å}}{\sqrt{3}} = 2.03\text{Å} \rightarrow$$

$$\theta = \sin^{-1}\left(\frac{\lambda}{2d_{hkl}}\right) = \sin^{-1}\left(\frac{2\text{Å}}{2 \cdot 2.03\text{Å}}\right) = 29.5^\circ$$

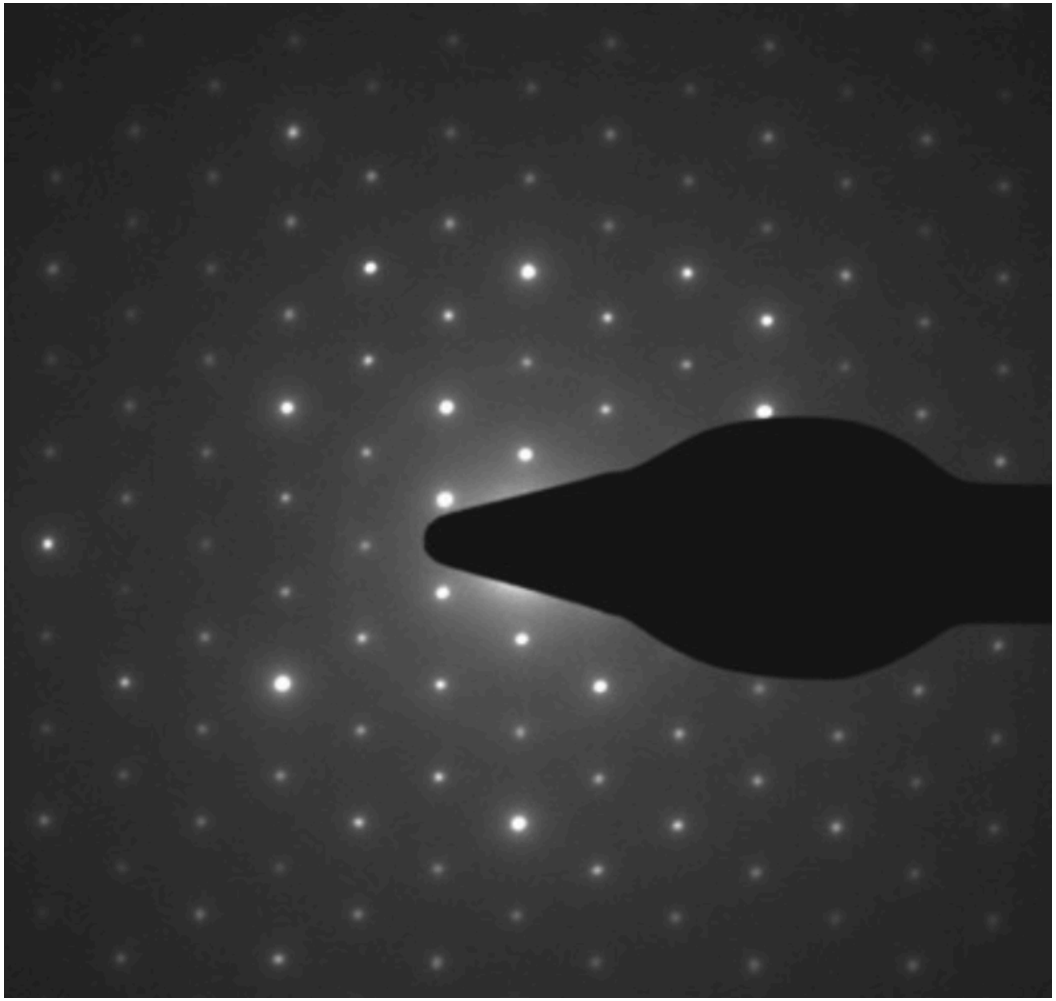
Different scattering angles from different planes



Different combinations of d and θ become relevant as the beam / crystal / detector change in orientation with respect to one another

Diffraction patterns

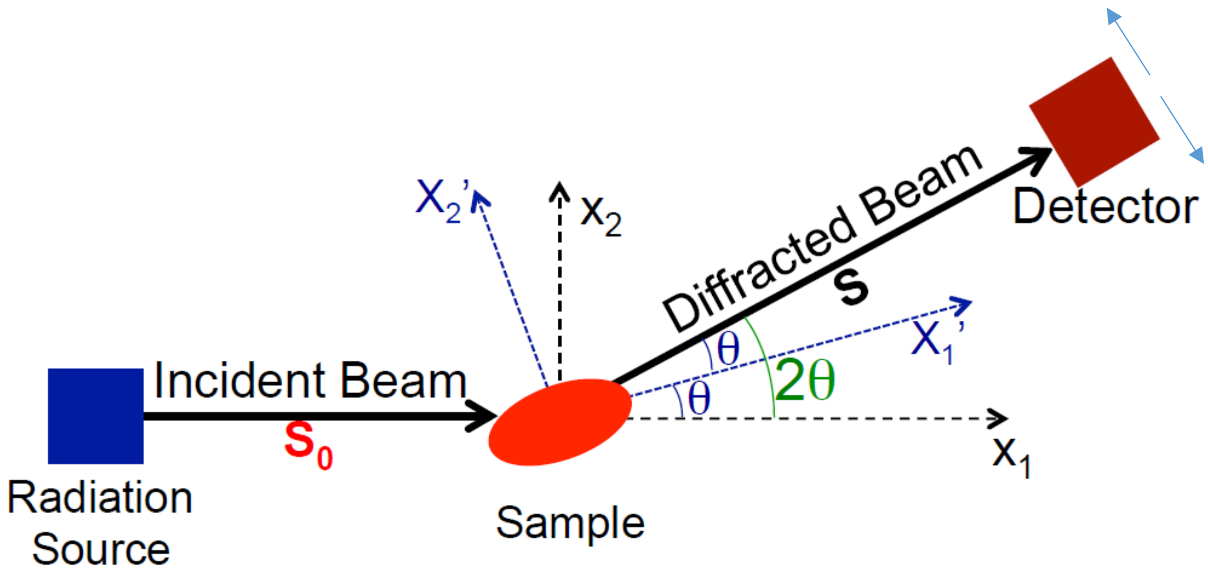
Diffraction pattern from single crystal Au (via TEM)

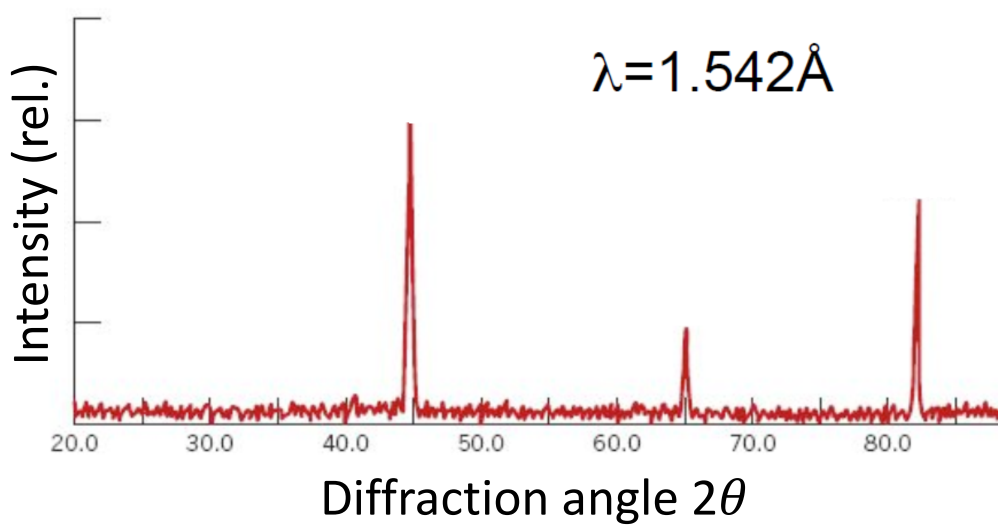


Lobastov et al., *PNAS* 2005; 102:7069.

Diffraction patterns

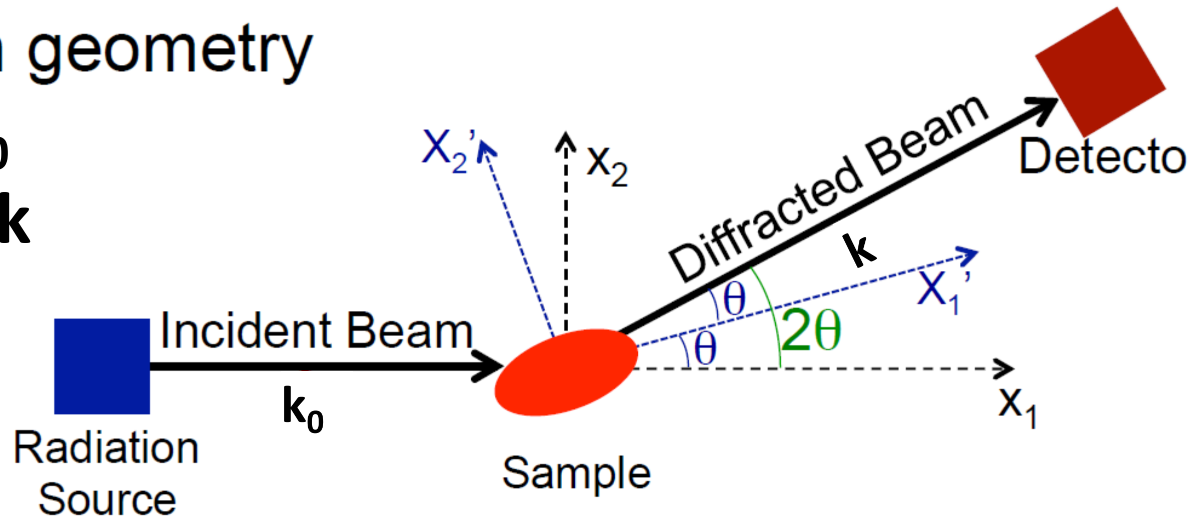
X-ray diffraction





Diffraction and the reciprocal lattice

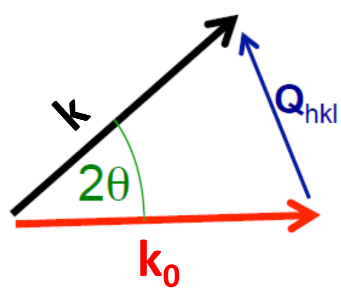
- Typical diffraction geometry
- Incident beam, $\mathbf{k_0}$
- Diffracted beam, $\mathbf{k}$
- $|\mathbf{k}|=|\mathbf{k_0}|=1/\lambda$

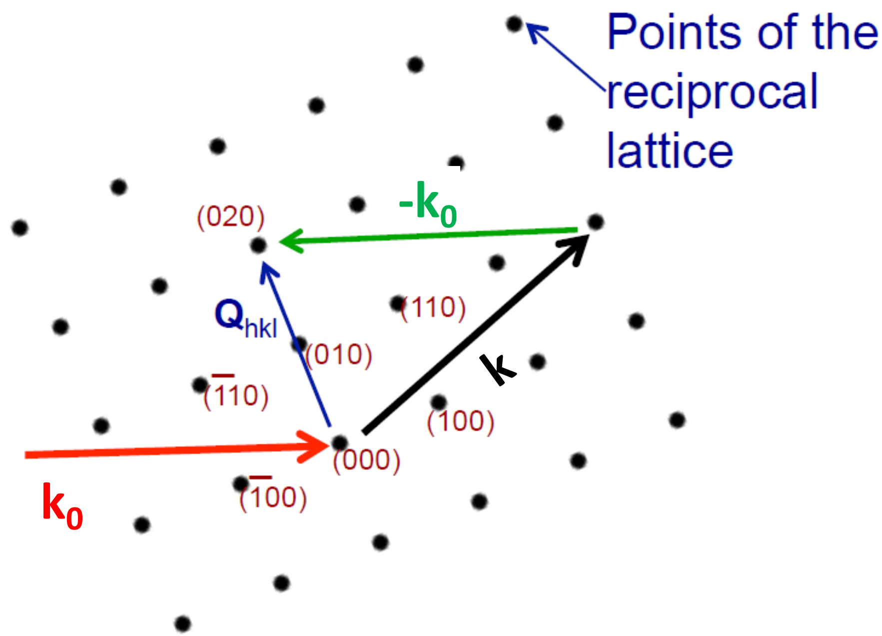


- Can rewrite Bragg's law as:

$$\Delta \mathbf{k} = \mathbf{k} - \mathbf{k_0} = \mathbf{Q}_{hkl}$$

Bragg condition:
reflection iff $\mathbf{k}-\mathbf{k_0}$ points to a reciprocal lattice point





The reciprocal lattice

- The reciprocal lattice describes plane normals. **Each point in the reciprocal lattice represents a set of diffracting real lattice planes.**
- Each crystal has both a real and a reciprocal lattice
- The "real" lattice is what you would expect to see if you zoom in very far with a microscope
- The "reciprocal" lattice is what you see in a diffraction pattern
- We define reciprocal lattice vectors $\mathbf{a_1}$*, $\mathbf{a_2}$*, and $\mathbf{a_3}$* corresponding to the real lattice vectors $\mathbf{a_1}$, $\mathbf{a_2}$, and $\mathbf{a_3}$:

$$\mathbf{a}_1^* = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}$$

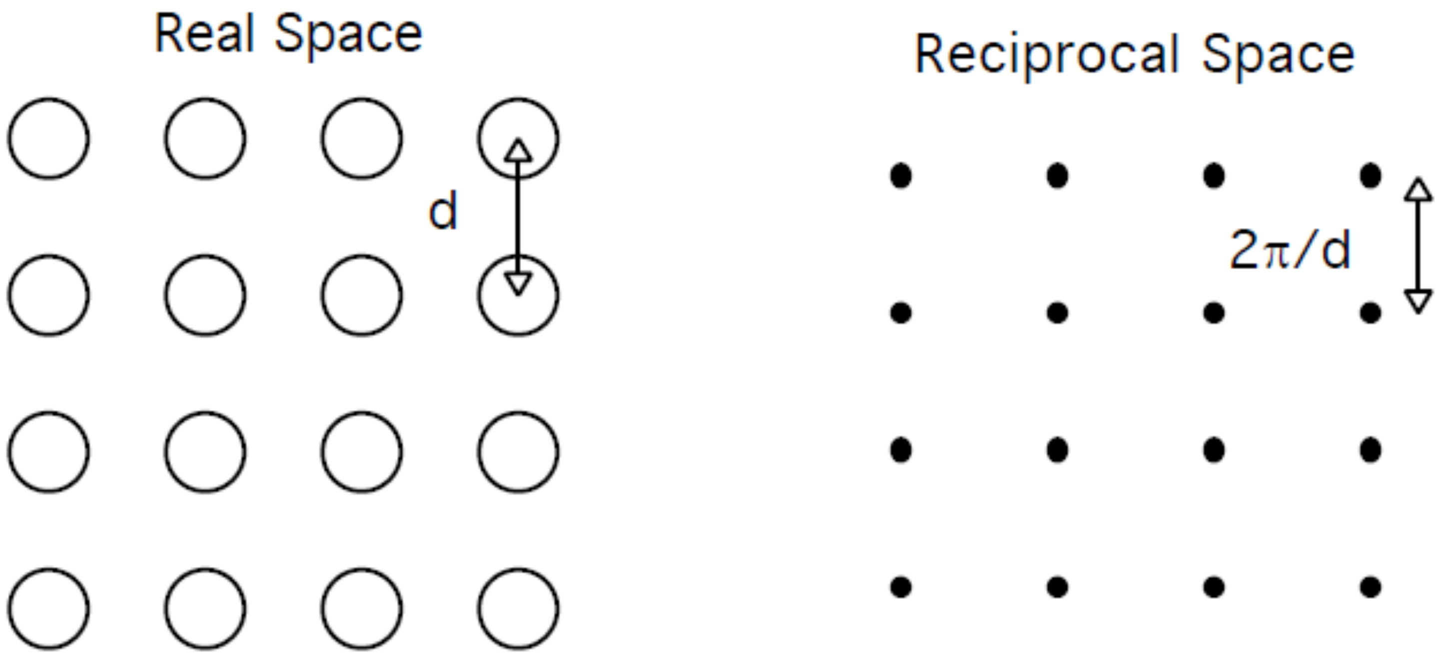
$$\mathbf{a}_2^* = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot \mathbf{a}_3 \times \mathbf{a}_1}$$

$$\mathbf{a}_3^* = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot \mathbf{a}_1 \times \mathbf{a}_2}$$

$$\mathbf{a}_i^* \cdot \mathbf{a}_j = \delta_{ij}$$

- And we can define the reciprocal lattice $Q_{hkl} = h\mathbf{a_1}^* + k\mathbf{a_2}^* + l\mathbf{a_3}^*$ for integers *h*, *k*, and *l*

Reciprocal lattice

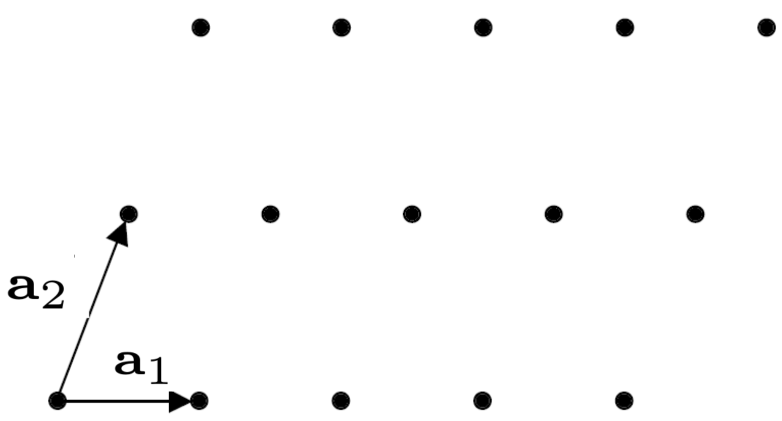


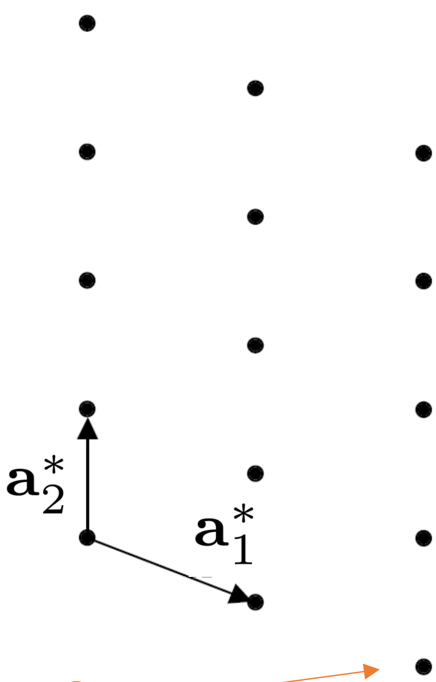
In the reciprocal lattice, the lattice points are spaced according to $k = 2\pi/d$ rather than by d

Example

Real space lattice $\mathbf{a}_1 = 2\hat{x}$, $\mathbf{a}_2 = \hat{x} + 2\hat{y}$, $\mathbf{a}_3 = \hat{z}$

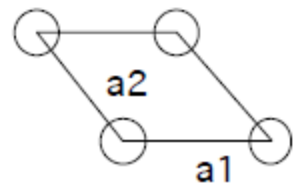
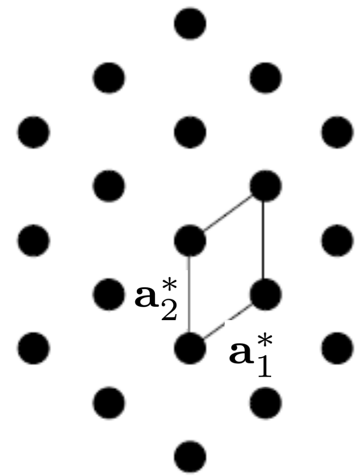
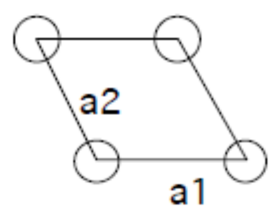
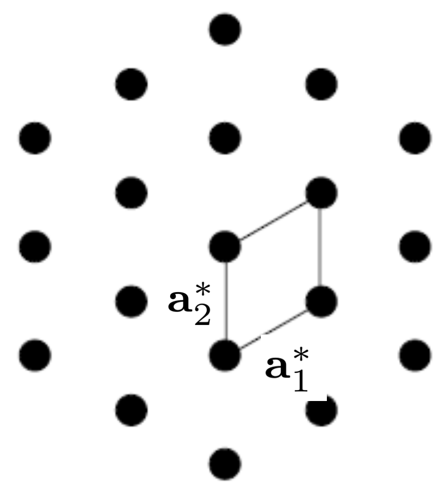
Reciprocal space lattice $\mathbf{a}_1^* = \dfrac{-\hat{y} + 2\hat{x}}{4}$, $\mathbf{a}_2^* = \dfrac{\hat{y}}{2}$, $\mathbf{a}_3^* = \hat{z}$



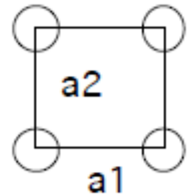
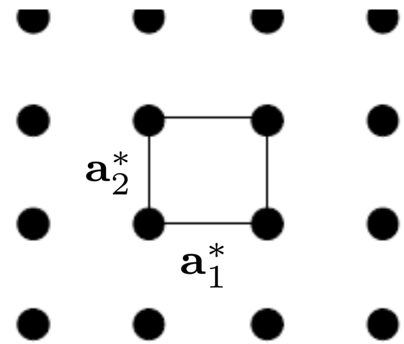
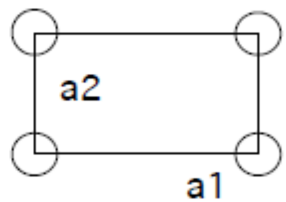
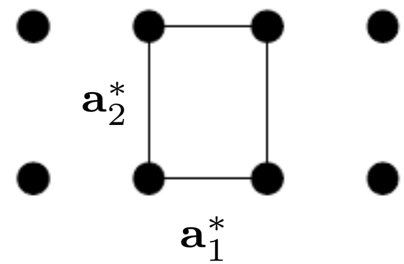


What does each point represent?

Reciprocal lattice

Lattice	Plane Lattice	Diffraction Pattern
Oblique (general)		
Hexagonal		

Reciprocal lattice

Lattice	Plane Lattice	Diffraction Pattern
Square		
Rectangular		
Centered Rectangular