Analytical Methods for Materials

Lesson 17

Interaction Between X-rays and Matter

Suggested Reading

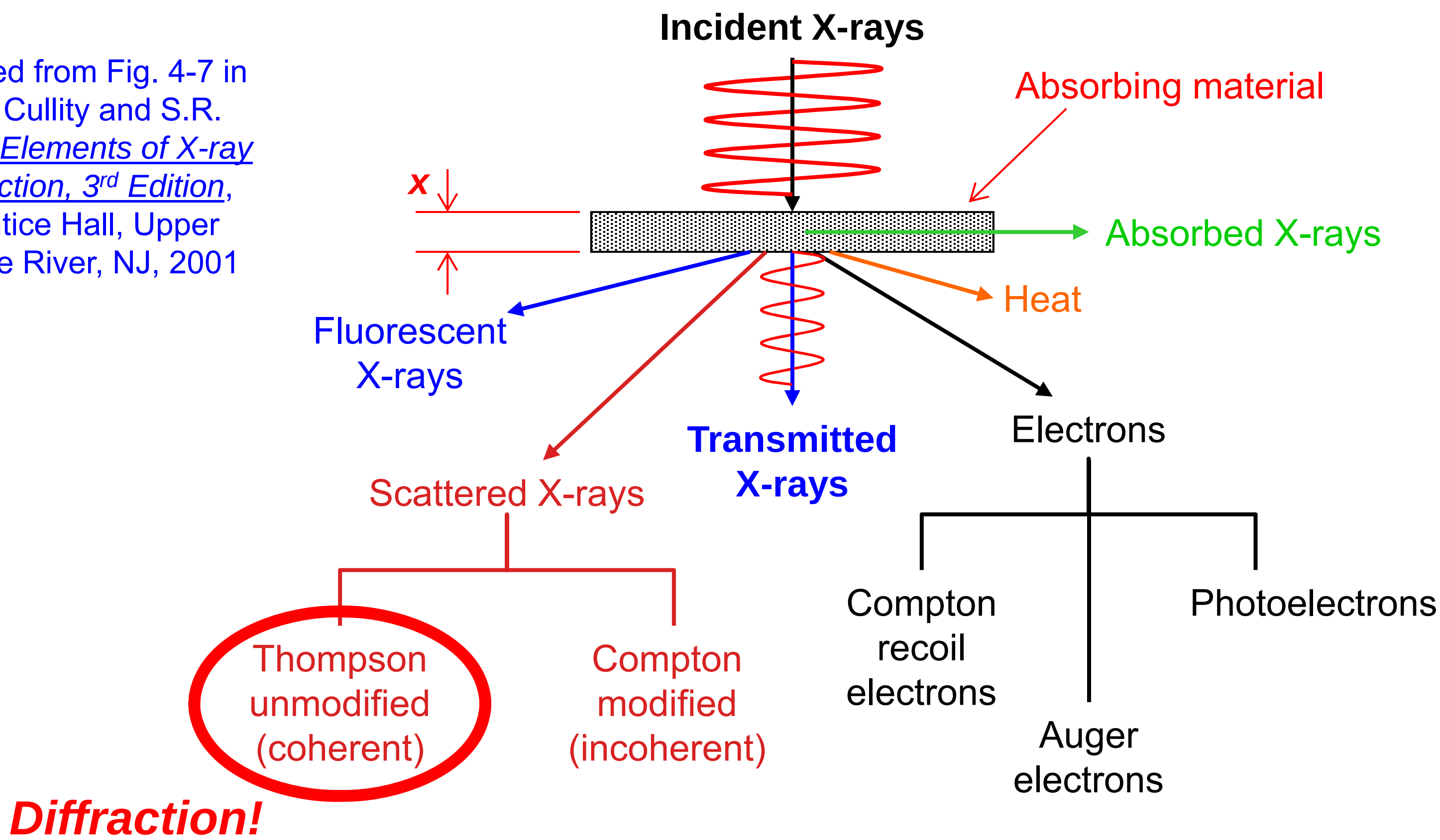
► Chapter 3 in Waseda, pp. 76-99

- Chapter 7 in Pecharsky and Zavalij
- Chapters 3 and 4 in Cullity & Stock
- Chapters 11 and 12 in De Graef & McHenry
- http://www.ndt-ed.org/EducationResources/educationresource.htm

RECALL

What happens when x-rays encounter matter?

Adapted from Fig. 4-7 in B.D. Cullity and S.R. Stock, *Elements of X-ray Diffraction, 3rd Edition*, Prentice Hall, Upper Saddle River, NJ, 2001



X-rays are ***attenuated***

Part of incident X-ray energy is lost as they travel through a material

X-ray Scattering

- X-ray is deflected from its original path with or without energy loss.
- Scattering occurs in all directions; thus, energy in the scattered is subtracted from the transmitted beam.
- There are two types.

Types of Scattering

1. Coherent (Thompson) scattering
   (*i.e.*, diffraction)

2. Incoherent (Compton) scattering

Coherent (Thompson) scattering

- Phase change due to difference in distance traveled.
- Scattered wave has a definite phase relationship w/ incident wave (i.e. $\phi = n\lambda$ where n is an integer).
- Scattered wave has the same λ as the incident wave.
- Leads to diffraction peaks.

Incoherent Scattering (Compton scattering)

- Phase change due to difference in distance traveled.
- There's an energy and momentum change during interaction.
- Change in λ.
- Thus, no phase relationship between the incoming and outgoing radiation (i.e. $\phi \neq n\lambda$).

Now let's consider things in a little more detail.

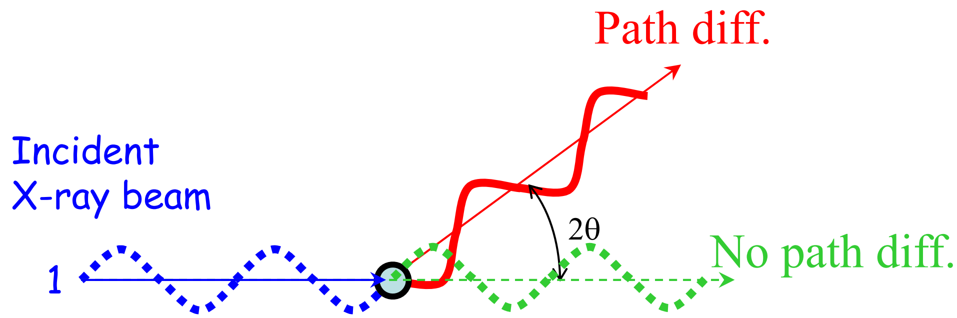
Scattering of X-rays by Atoms

- X-rays are scattered by electrons.
- Electron positions are determined by atom positions.
- Therefore:

  1) Size an shape of unit cell determine position of diffracted beam and

  2) Atom position determines the intensity of the diffracted beam.

Scattering by a single electron



- May be elastic* – no energy loss (or λ change)
  - Phase relationship between incident and scattered X-ray. $\phi = n\lambda$
- May be inelastic¥ – energy loss
  - No phase relationship between incident and scattered X-ray. $\phi \neq n\lambda$

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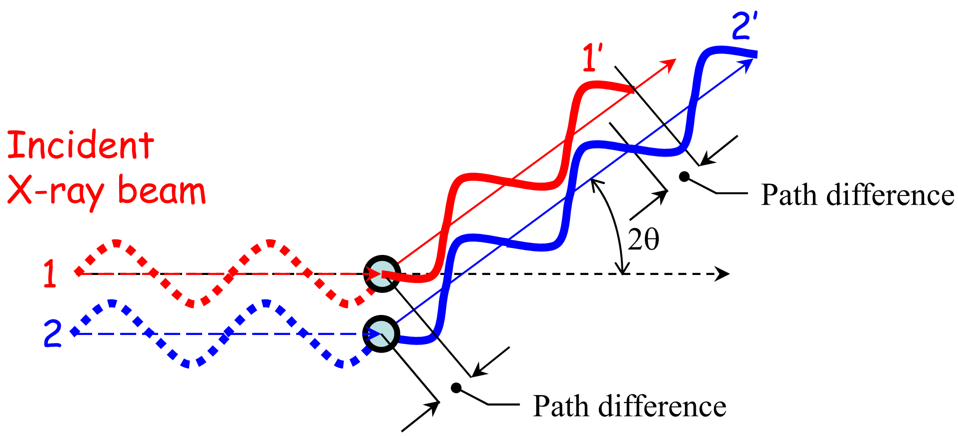
* Thompson scattering. Leads to strong XRD peaks

¥ Compton scattering. Leads to weak XRD peaks

Scattering by multiple electrons

[Ref. Coherent scattering]



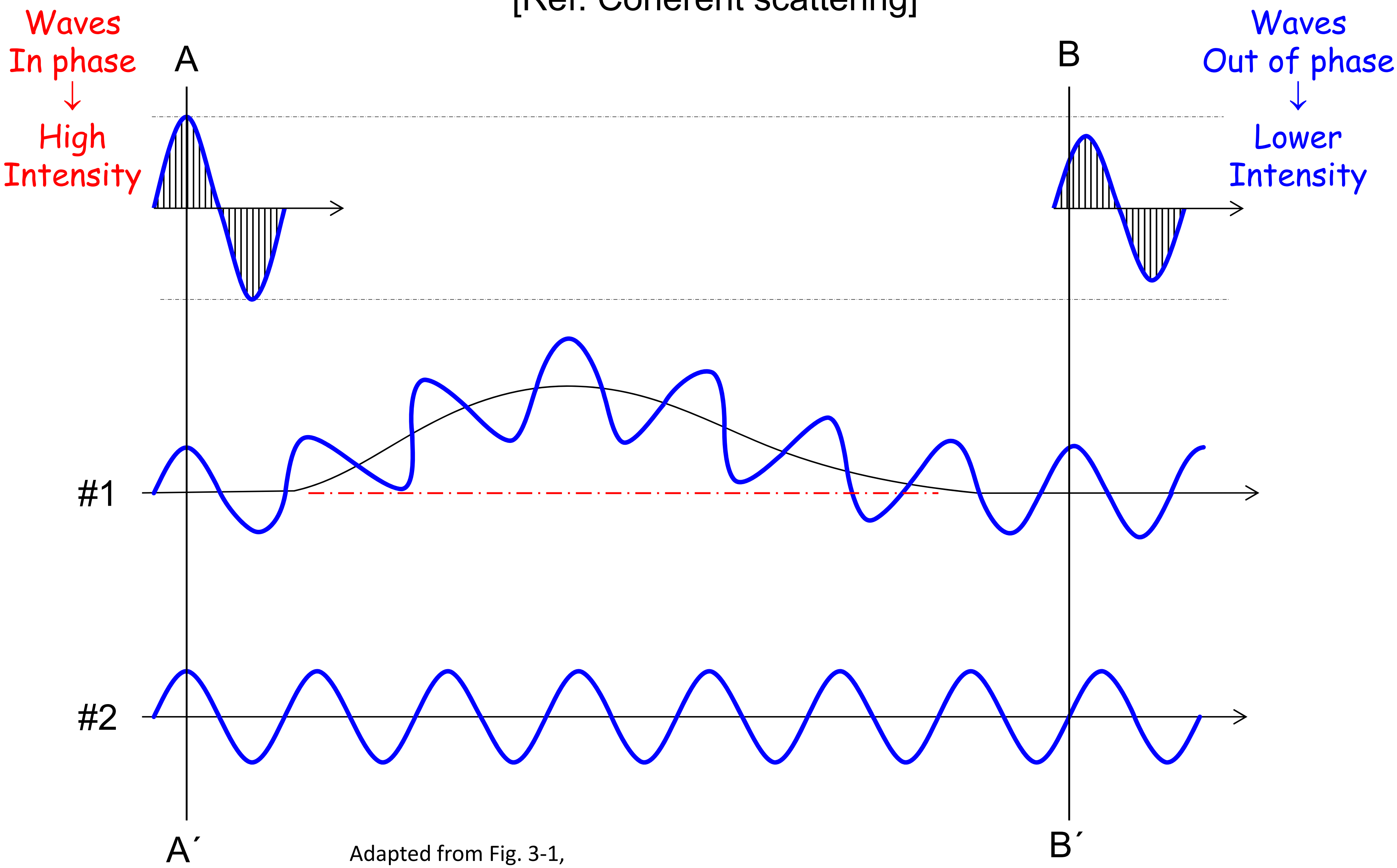
- With Thompson scattering, a difference in path traveled can lead to reduced X-ray intensity.

$$\Sigma(1+2) > \Sigma(1'+2')$$

- However, when path difference = $n\lambda$, where n is an integer, intensity will be maximum.
- See the next viewgraph.

Effect of Path Difference on Phase

[Ref. Coherent scattering]



Adapted from Fig. 3-1,
Cullity & Stock, 3e.

Scattering by a single atom

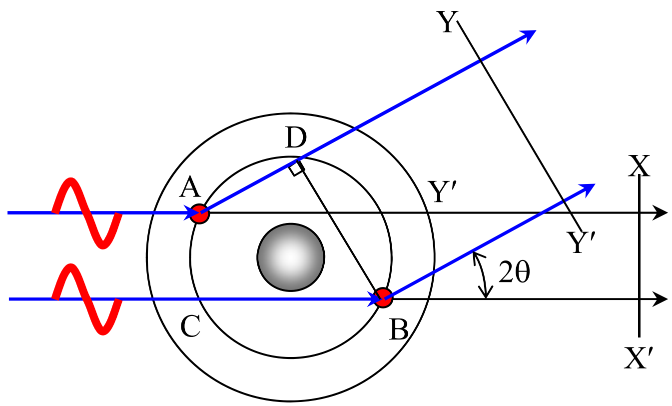
- Consider scattering by two e^- in an atom.

[Ref. Coherent scattering]

Just an extension of scattering by electrons

- The path difference for each photon is:

$$\delta = \mathrm{CB} - \mathrm{AD}$$



x-rays are scattered by electrons

- Path difference leads to a <u>difference in phase</u> between the two waves:

$$\phi = \frac{\delta}{\lambda} \times 2\pi \quad \text{(radians)}$$

- Scattered waves will not be in phase across wavefront YY′ unless $\delta = n\lambda$.

Additional Comments About Scattering

[Ref. Incoherent scattering]

- Incoherent scattering (i.e., Compton modified scattering) also occurs along with coherent scattering.
- Compton scattering results in a loss in photon energy in the scattered beam which ↑ λ.
- Leads to a loss in intensity of the scattered wave and increased background.

Additional Comments About Scattering

[Ref. Incoherent scattering]

- Compton scattering arises from collisions of quanta with loosely bound electrons.
  - Electrons are more loosely bound in low atomic number elements.
  - The intensity of Compton modified radiation increases as the atomic number (Z) decreases.
- This makes X-ray diffraction signals weaker in low Z materials.

Atomic Scattering Factor

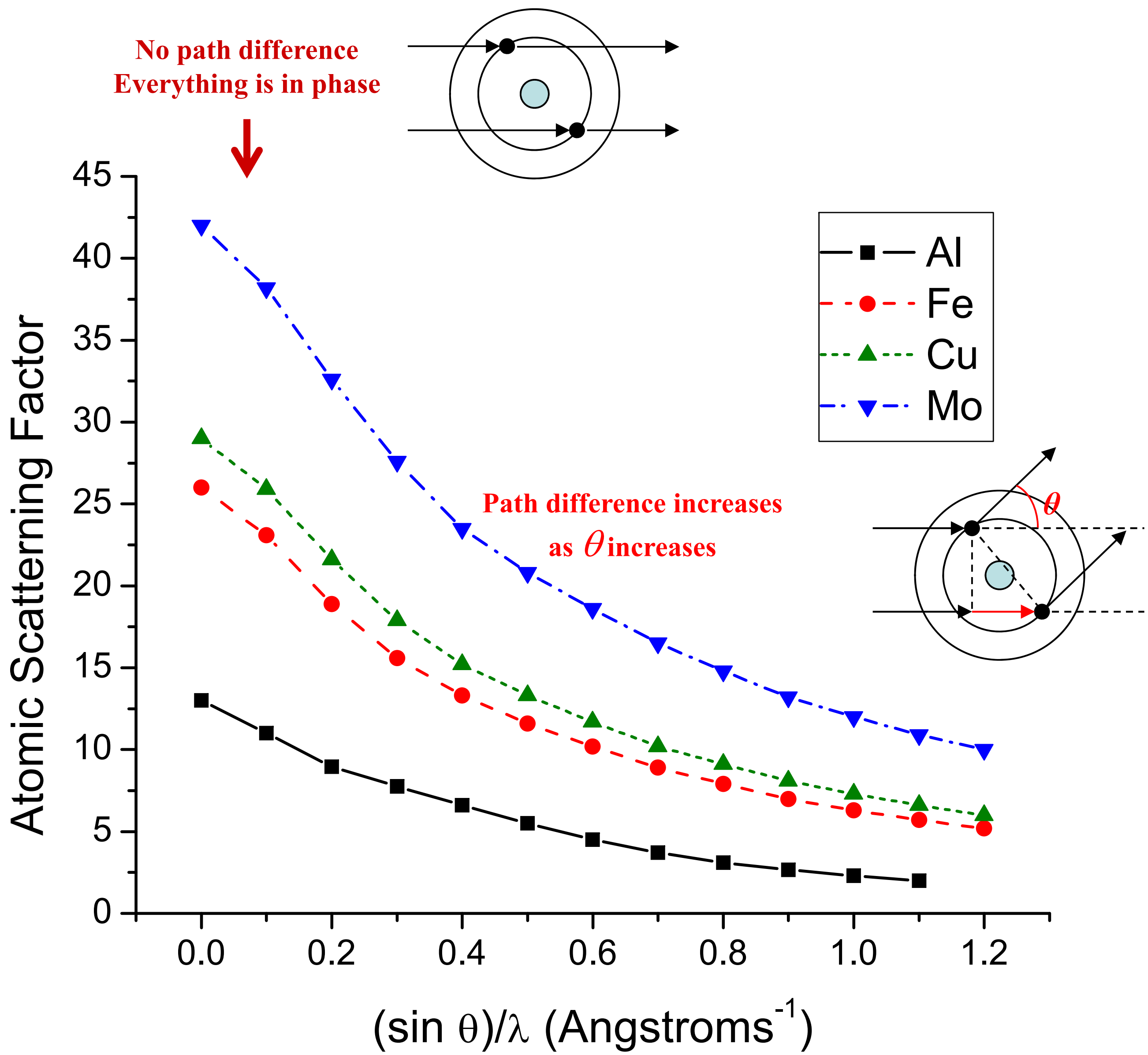
- Describes how efficiently an atom is scattering in a given direction.

$$f = \frac{\text{Amplitude of wave scattered by an atom}}{\text{Amplitude of wave scattered by one electron}}$$

- $f = \mathrm{Z}$ at $2\theta = 0^{\mathrm{o}}$; corresponds to forward scattering ("all electrons work together").

Variation of the atomic scattering factor with (sinθ)/λ for Al, Fe, Cu, and Mo.

You will find tabulated values for all elements in X-ray reference books.



- As θ increases, *f* decreases. **WHY?**
- As *λ* decreases, *f* decreases. **WHY?**

Answers

- As θ increases, f decreases. **WHY?**

As θ increases, the waves scattered by individual electrons get more out of phase (i.e., ϕ increases).

- As λ decreases, f decreases. **WHY?**

At fixed θ, path differences δ become larger relative to λ leading to more interference between scattered beams.

Diffraction

- X-rays scattered by multiple atoms will interact.
  - They are coherent if they are in phase (i.e., they reinforce each other).
  - Coherent X-rays "interfere" constructively.
- The directions in which the waves diffract depends on:
  - The wavelength (λ) of the incident radiation;
  - Atomic arrangement (i.e., crystal structure) of the sample.
  - Microstructure of sample.

Interference and Diffraction

[Restating the obvious]

- For closely spaced planes of atoms, scattered waves reinforce <u>or</u> cancel.

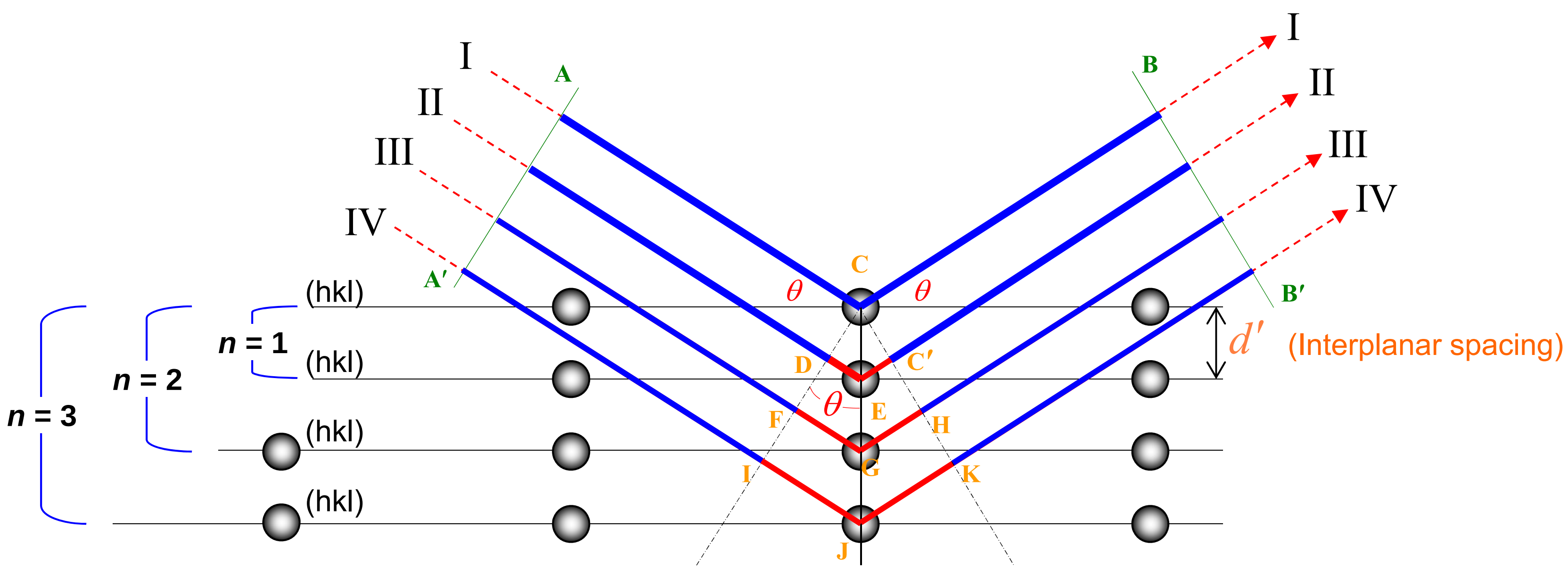
- **<u>Constructive</u> <u>interference</u>:** waves are in phase leading to a strong signal (*i.e.*, big resultant wave).

- **<u>Destructive</u> <u>interference</u>:** waves are out of phase leading to a reduced or nonexistent signal.

SCATTERING BY A CRYSTAL

[Let's relate things back to Bragg's Law]

- Derivation based on a parallel monochromatic, coherent (in phase) incident beam.



- For all waves to be in phase, their collective path differences (δ) must be equal to an integral number of wavelengths

(i.e., $\delta = n\lambda$)

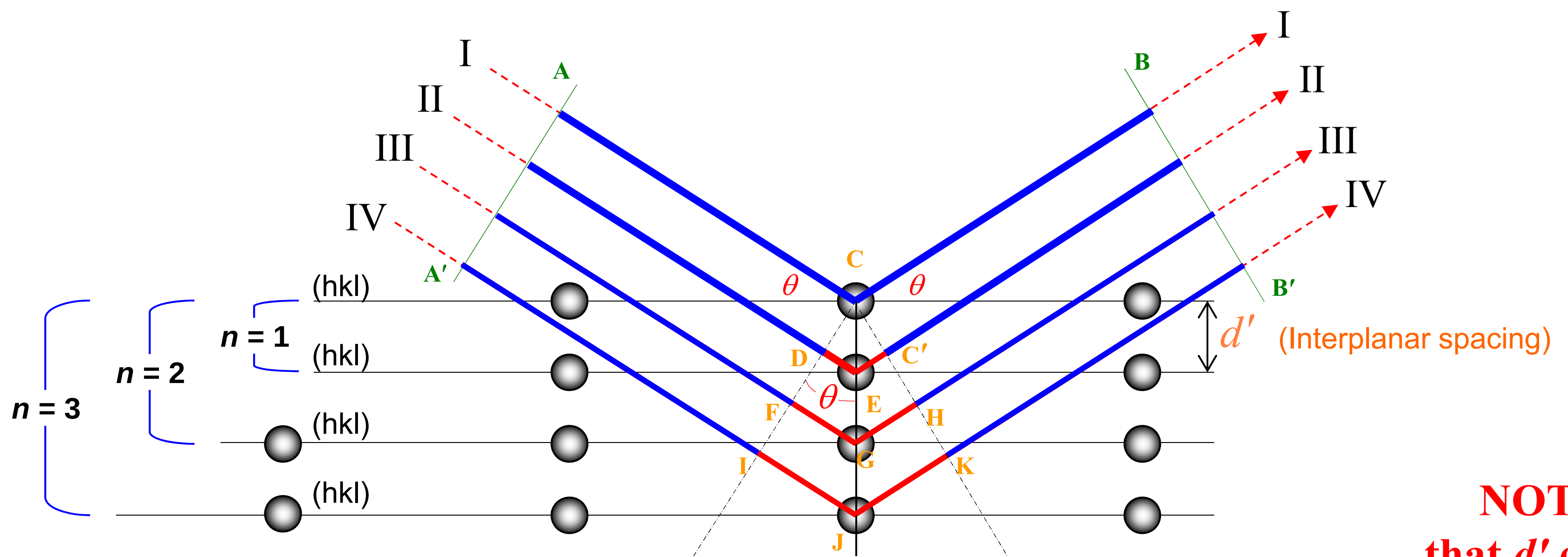
[Referring to the diagram on the previous page]

When waves I and II are in phase

$$\mathrm{DE} + \mathrm{EC}' = \delta = n\lambda$$

$$\boxed{n\lambda = 2d' \sin\theta}$$ ***Bragg's Law***

For multiple waves diffracted by parallel atomic planes



NOTICE
that d' changes

$$\boldsymbol{\delta = n\lambda}\text{, where } n = \text{whole number}$$

$\boldsymbol{n = 1}$: $\delta_{I\rightarrow II} = 1\lambda = DE+EC' = CE\sin\theta + CE\sin\theta = 2d'\sin\theta$

$\boldsymbol{n = 2}$: $\delta_{I\rightarrow III} = 2\lambda = FG+GH = CG\sin\theta + CG\sin\theta = 2(2d')\sin\theta$

$\boldsymbol{n = 3}$: $\delta_{I\rightarrow IV} = 3\lambda = IJ+JK = CJ\sin\theta + CJ\sin\theta = 2(3d')\sin\theta$

$\boldsymbol{n = n_i}$: $\delta_{I\rightarrow i} = n_i\lambda = 2(n_i d')\sin\theta$

n is the order of diffraction

- $n = 1$, path difference $\delta = \lambda$ **1st order**
- $n = 2$, path difference $\delta = 2\lambda$ **2nd order**
- $n = 3$, path difference $\delta = 3\lambda$ **3rd order**
- $n = 4$, path difference $\delta = 4\lambda$ **4th order**
- *Etc.*

Scattering Modes

- Atoms arranged randomly in space (e.g., a gas or liquid)
  - Scattering/diffraction is in all directions.
    Small diffraction peaks (if any).

- Atoms arranged in regular patterns (e.g., crystal)
  - In some directions (when Bragg's law is satisfied) scattering/diffraction is strong. Big diffraction peaks.
  - In directions that do not satisfy Bragg's law, there is no scattering

- We can re-write Bragg's law as:

$$\lambda = 2\frac{d'}{n}\sin\theta$$

- d' = spacing between planes (hkl)

- d'/n = spacing between planes ($nh\ nk\ nl$)

- Let $d = d'/n$ and we can write Bragg's law as:

$$\lambda = 2d_{hkl}\sin\theta$$

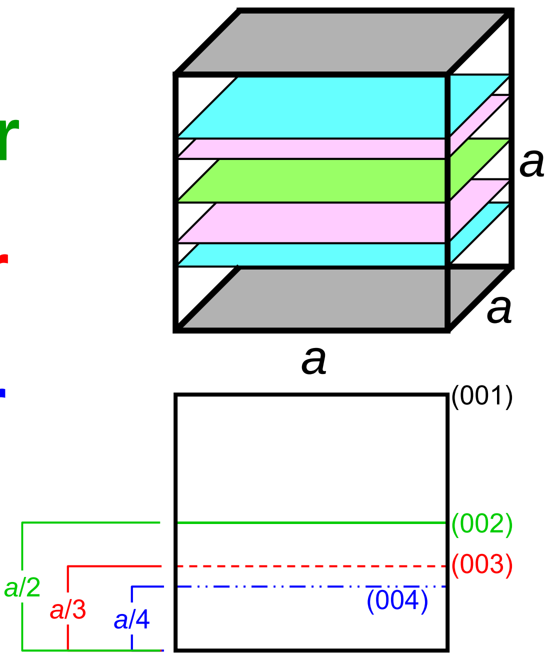
Allows us to consider reflections of any order as first order reflections from planes spaced at a distance 1/*n* of the previous spacing.

n = order of diffraction

EXAMPLE

(001)

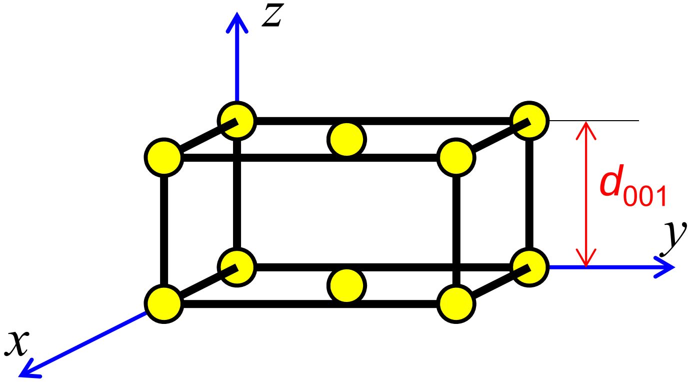
- $n = 1$, (001) $\delta = \lambda$ **1st order**
- $n = 2$, (002) $\delta = [1/2]\lambda$ **2nd order**
- $n = 3$, (003) $\delta = [1/3]\lambda$ **3rd order**
- $n = 4$, (004) $\delta = [1/4]\lambda$ **4th order**
- *Etc.*

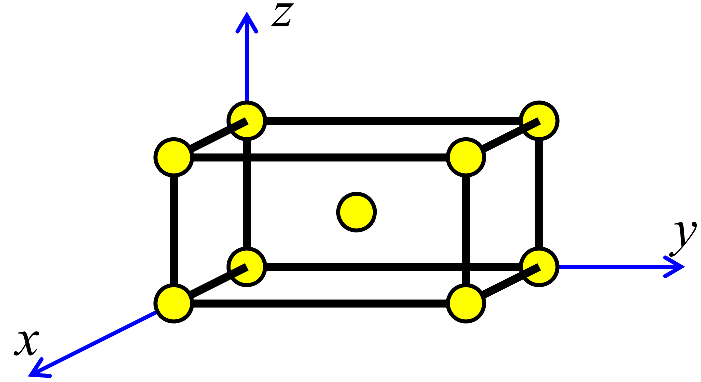


Now let's consider how atom placement on a plane influences the diffracted beam

Intensity of Diffracted Beams

- The type of unit cell influences the intensity of the diffracted beam but not the direction of the diffracted beam.



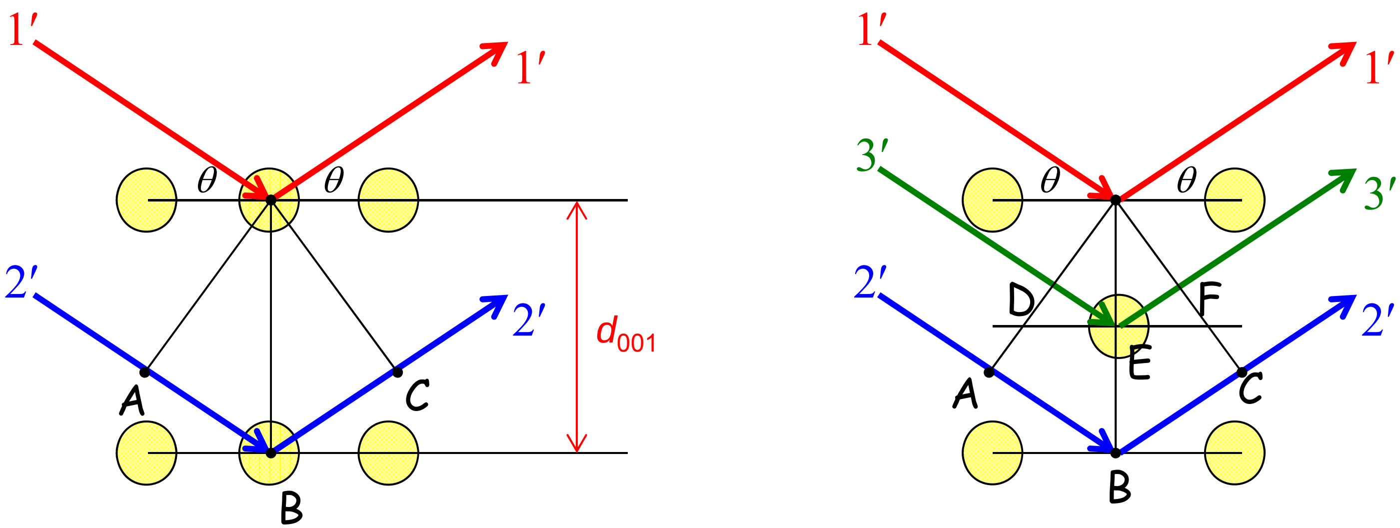


Consider the base-centered and body-centered orthorhombic unit cells drawn above.

WHAT HAPPENS IF WE DIFFRACT X-RAYS FROM THE (001) PLANES OF EACH?

[consider all orders]

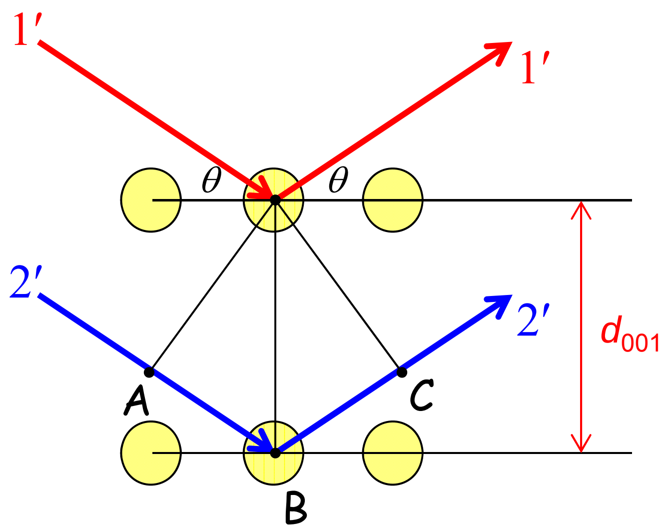
Diffraction from (001)

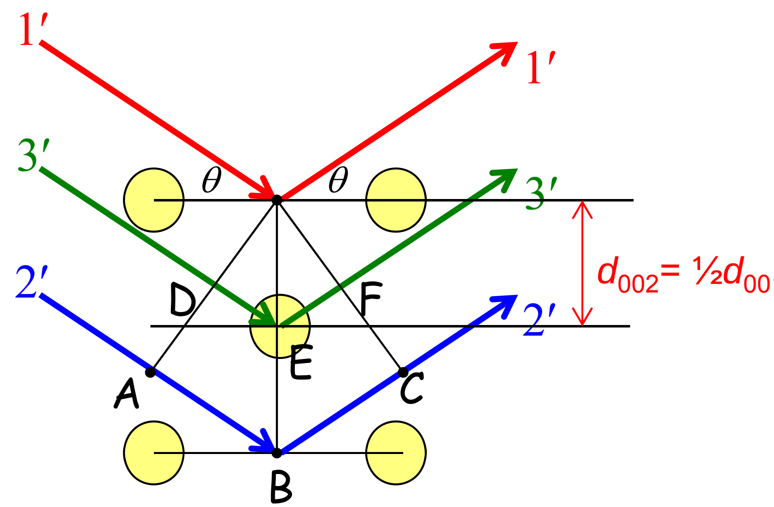


In Both Unit Cells

The path difference between rays 1′ and 2′, $\delta_{1'\text{-}2'}$ (*i.e.*, ABC) = 1λ (*i.e.*, one wavelength).

Diffraction from (001)





<u>In the Body Centered Unit Cell</u>

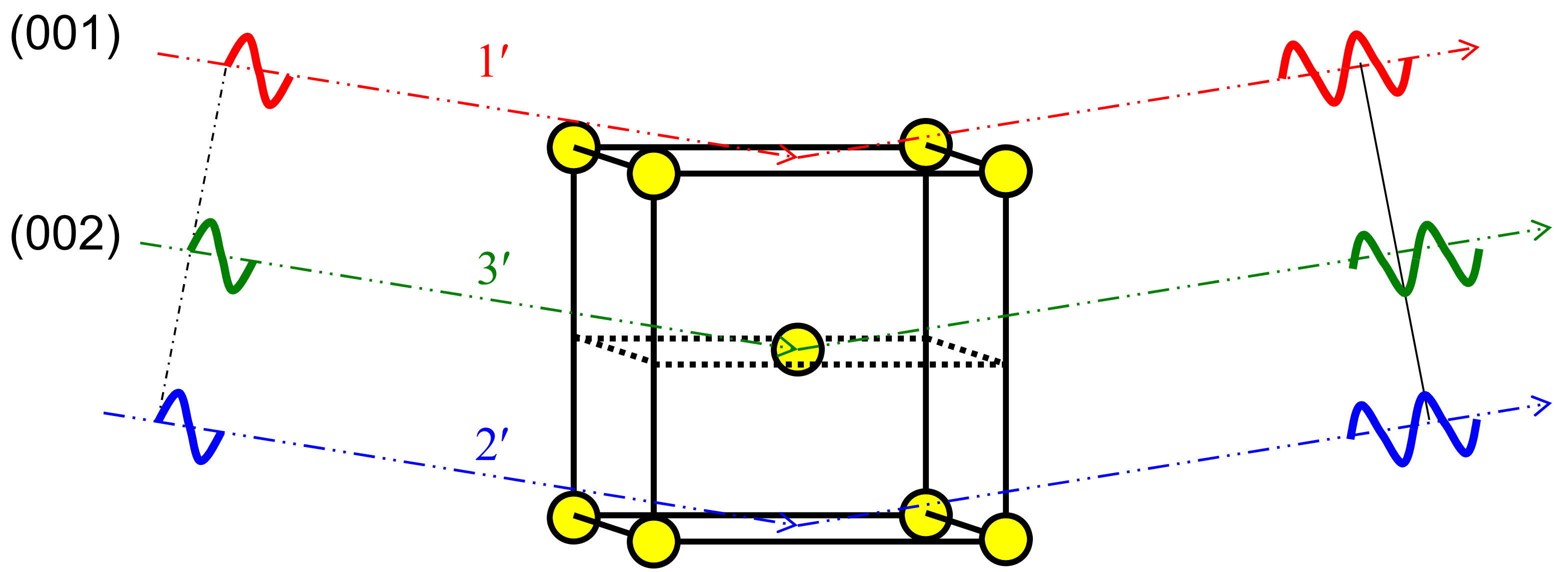
The path difference between rays 1′ and 3′,

$\delta_{1'\text{-}3'}$ (*i.e.*, DEF) = ½× $\delta_{1'\text{-}2'}$ (*i.e.*, one wavelength)

or

$\delta_{1'\text{-}3'}$ = ½× λ (*i.e.*, 180°)

IMPLICATIONS



- Diffracted waves from the (001) and (002) crystal planes are 180° out of phase and will cancel each other out.

- Thus, there will not be a (001) reflection in a body centered cell.

IMPLICATIONS – cont'd

- For some crystal structures certain reflections will be absent.

- They are called forbidden reflections.

- We can assess which reflections are allowed and which are forbidden via a structure factor calculation.