



# Analytical Methods for Materials

## Lesson 17

### Interaction Between X-rays and Matter

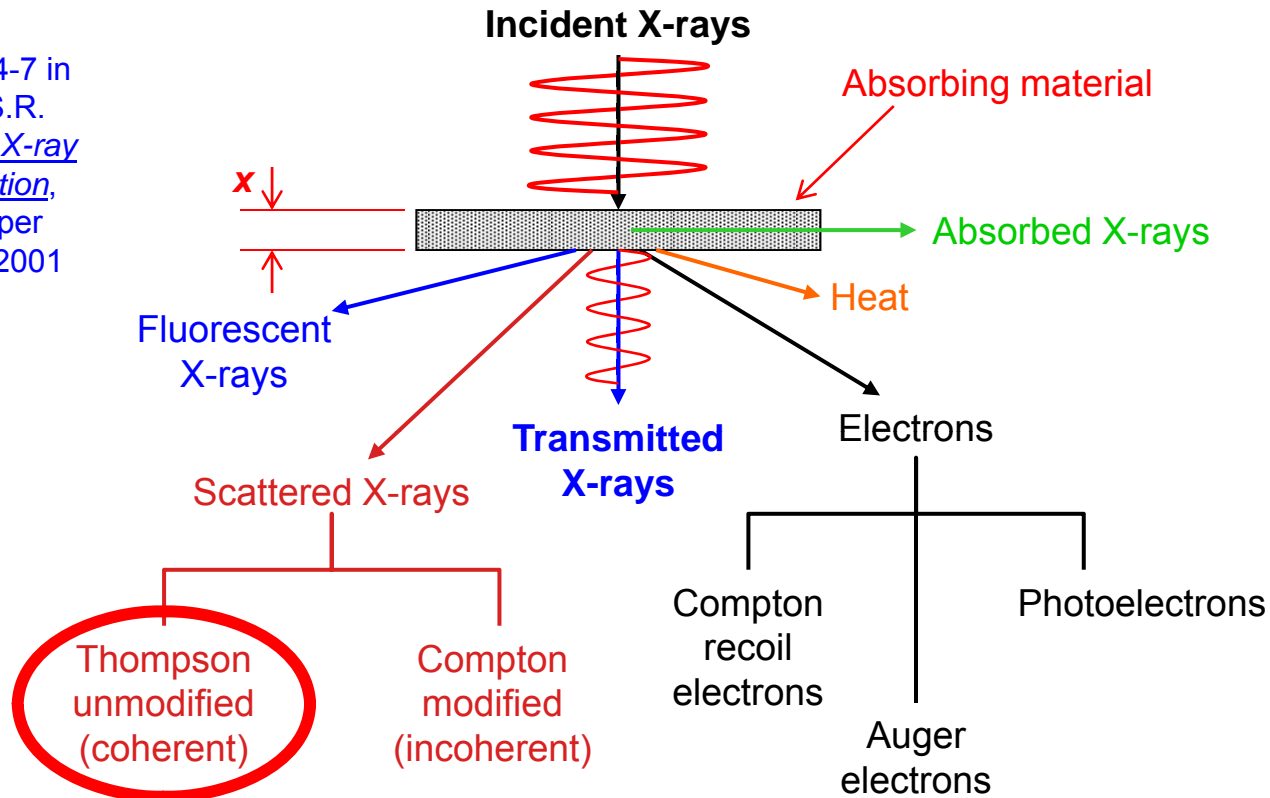
#### Suggested Reading

- ▶ 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, 3<sup>rd</sup> Edition*,  
Prentice Hall, Upper  
Saddle River, NJ, 2001



**Diffraction!**

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  $\lambda$  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  $\lambda$ .
- Thus, no phase relationship between the incoming and outgoing radiation (i.e.  $\phi \neq n\lambda$ ).

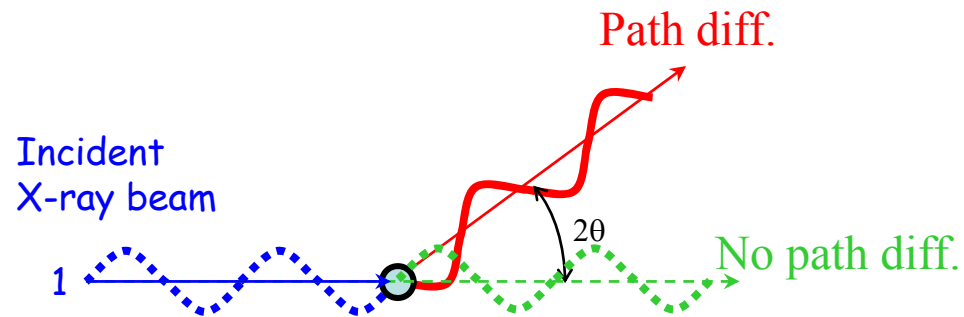
Now let's consider  
things in a little  
more detail.

# Scattering of X-rays by Atoms

- X-rays are scattered by electrons.
- Electron positions are determined by atom positions.
- Therefore:
  - 1) Size and 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  $\lambda$  change)
  - Phase relationship between incident and scattered X-ray.  $\phi = n\lambda$
- May be inelastic $\ddagger$  – energy loss
  - No phase relationship between incident and scattered X-ray.  $\phi \neq n\lambda$

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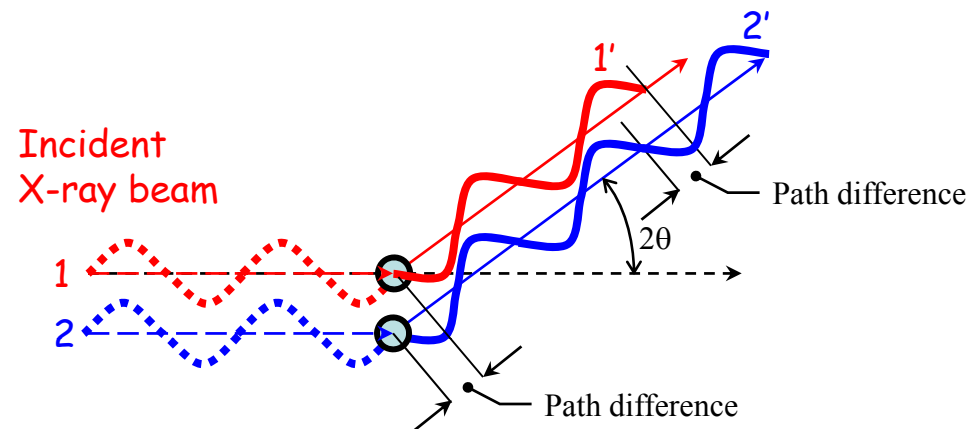
\* Thompson scattering. Leads to strong XRD peaks

$\ddagger$  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.

# Scattering by a single atom

- Consider scattering by two  $e^-$  in an atom.
- The path difference for each photon is:

$$\delta = CB - AD$$

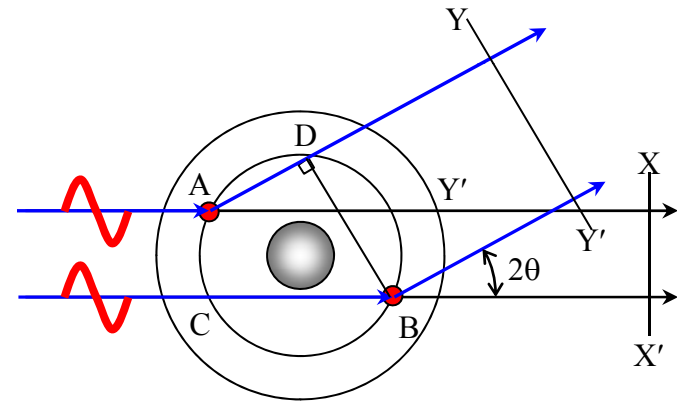
- Path difference leads to a difference in phase between the two waves:

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

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

[Ref. Coherent scattering]

**Just an extension  
of scattering by  
electrons**



x-rays are scattered by electrons

# 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  $\uparrow \lambda$ .
- Causes a loss in intensity of the scattered wave and increased background.

# Additional Comments About Scattering

[Ref. Incoherent scattering]

- Compton scattering results from collisions of quanta with loosely bound electrons.
- Electrons are more loosely bound in low atomic number elements.
- Thus, 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

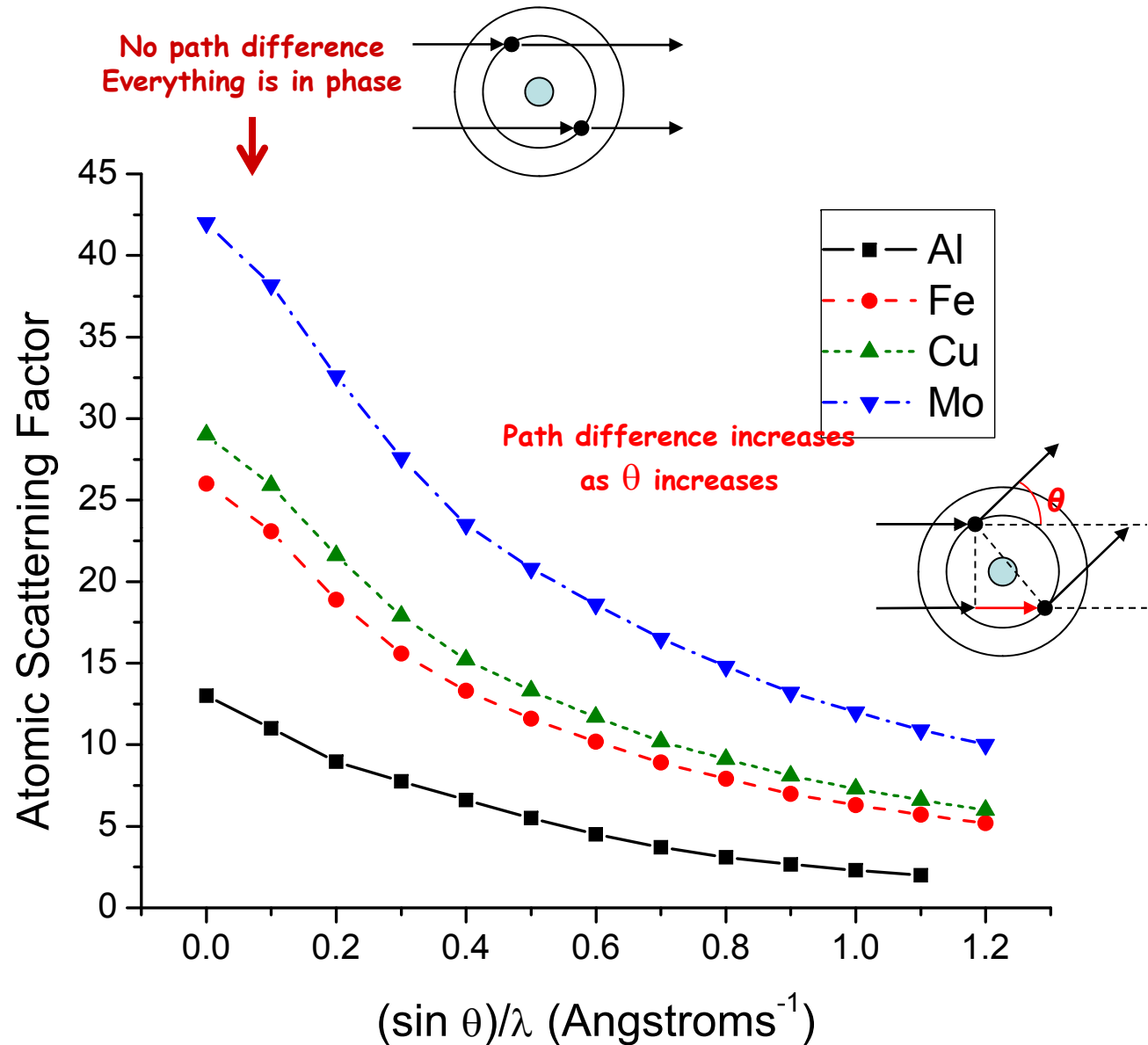
- Describes how efficiently an atom is scattering in a given direction.

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

- $f = Z$  at  $2\theta=0^\circ$ ; corresponds to forward scattering (“all electrons work together”).

Variation of the atomic scattering factor with  $(\sin\theta)/\lambda$  for Al, Fe, Cu, and Mo.

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



- As  $\theta$  increases,  $f$  decreases. **WHY?**
- As  $\lambda$  decreases,  $f$  decreases. **WHY?**

# Answers

- As  $\theta$  increases,  $f$  decreases. **WHY?**

- As  $\lambda$  decreases,  $f$  decreases. **WHY?**



# 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 ( $\lambda$ ) of the incident radiation;
  - Atomic arrangement (i.e., crystal structure) of the sample.
  - Microstructure of sample.

# Interference and Diffraction

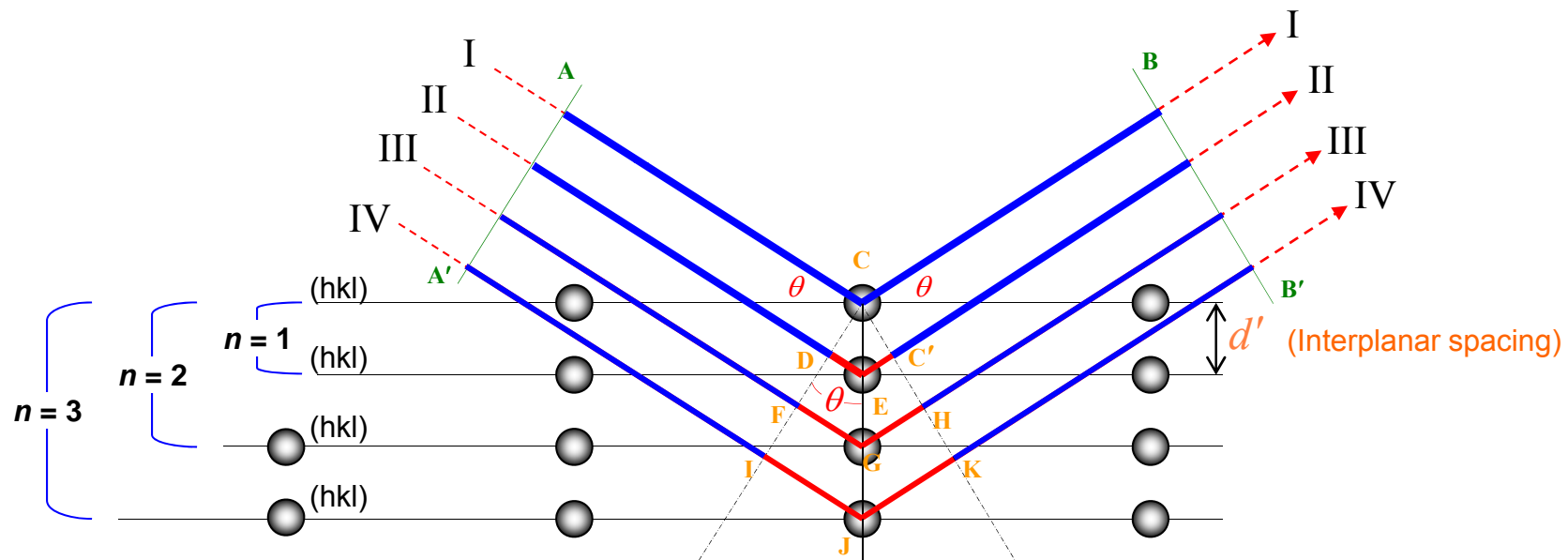
[Restating the obvious]

- For closely spaced planes of atoms, scattered waves reinforce or cancel.
- **Constructive interference**: waves are in phase leading to a strong signal (*i.e.*, big resultant wave).
- **Destructive interference**: 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 ( $\delta$ ) must be equal to an integral number of wavelengths

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

[Referring to the diagram on the previous page]

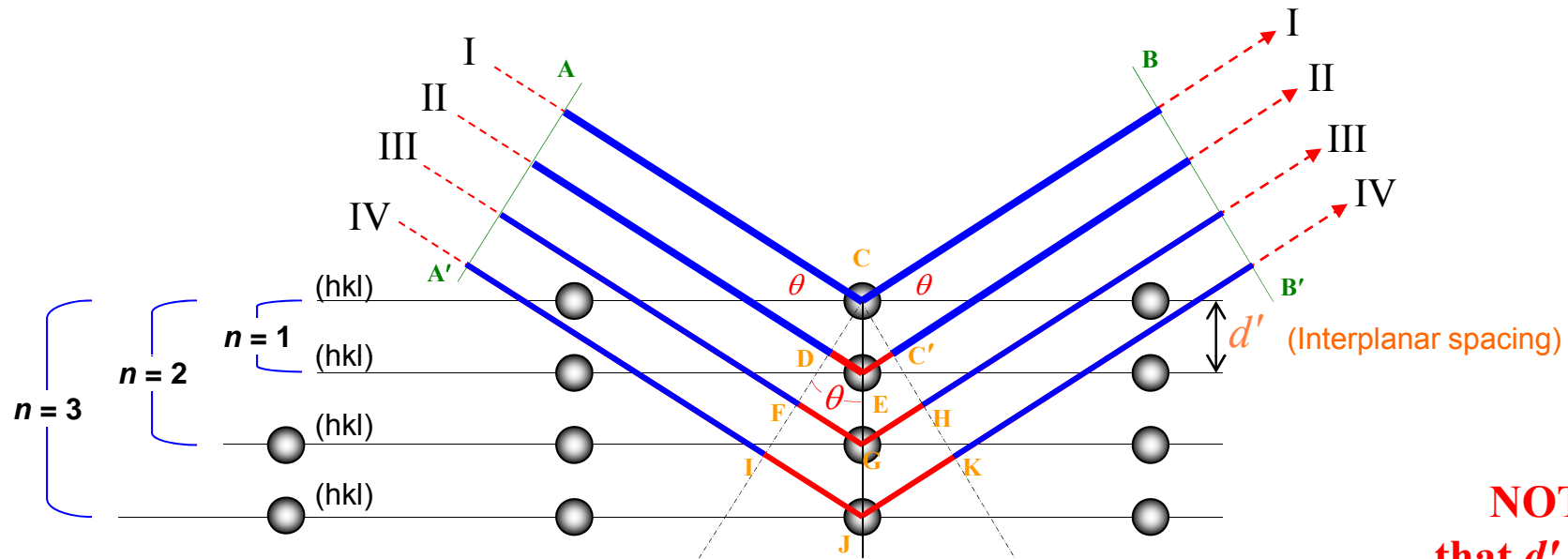
When waves I and II are in phase

$$DE + EC' = \delta = n\lambda$$

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

***Bragg's Law***

# For multiple waves diffracted by parallel atomic planes



**NOTICE**  
that  $d'$  changes

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

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

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

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

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

## **$n$ is the order of diffraction**

- $n = 1$ , path difference  $\delta = \lambda$  **1<sup>st</sup> order**
- $n = 2$ , path difference  $\delta = 2\lambda$  **2<sup>nd</sup> order**
- $n = 3$ , path difference  $\delta = 3\lambda$  **3<sup>rd</sup> order**
- $n = 4$ , path difference  $\delta = 4\lambda$  **4<sup>th</sup> 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:

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

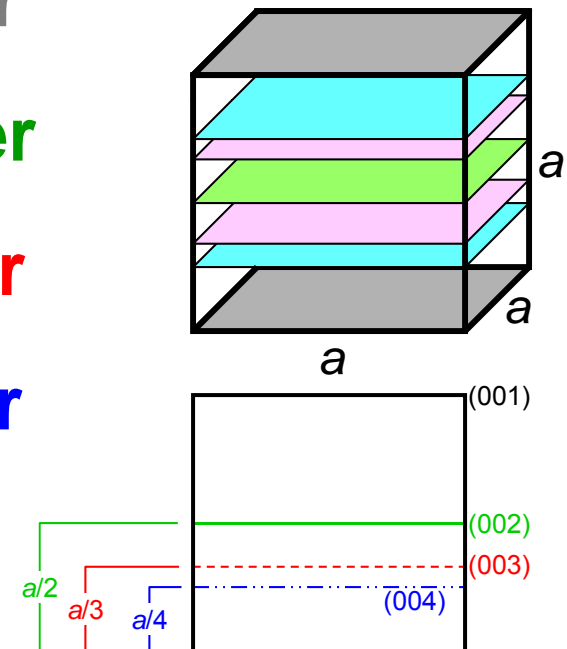
Allows us to consider reflections of any order as first order reflections from planes spaced at a distance  $1/n$  of the previous spacing.

## $n = \text{order of diffraction}$

### EXAMPLE

(001)

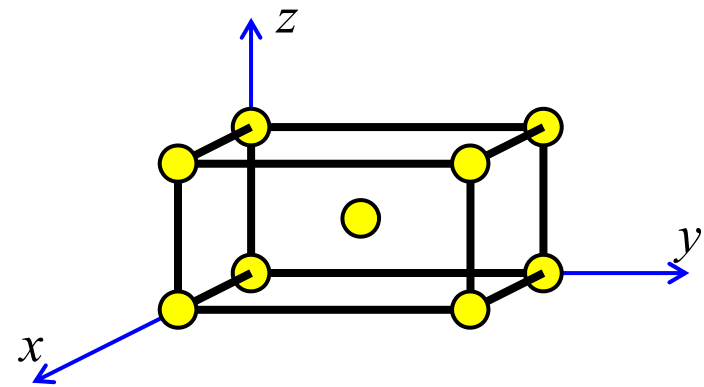
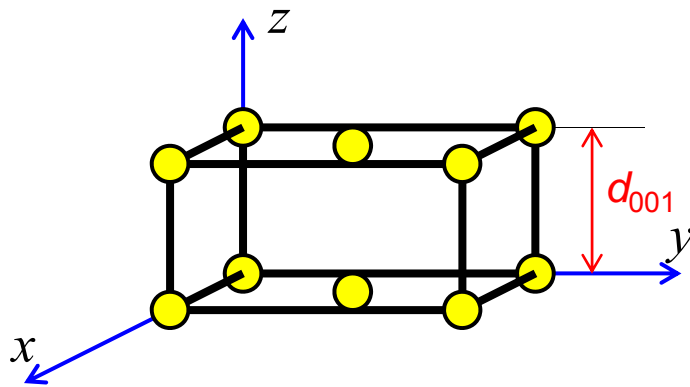
- $n = 1, (001) \delta = \lambda$       1<sup>st</sup> order
- $n = 2, (002) \delta = [1/2]\lambda$       2<sup>nd</sup> order
- $n = 3, (003) \delta = [1/3]\lambda$       3<sup>rd</sup> order
- $n = 4, (004) \delta = [1/4]\lambda$       4<sup>th</sup> order
- *Etc.*



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.

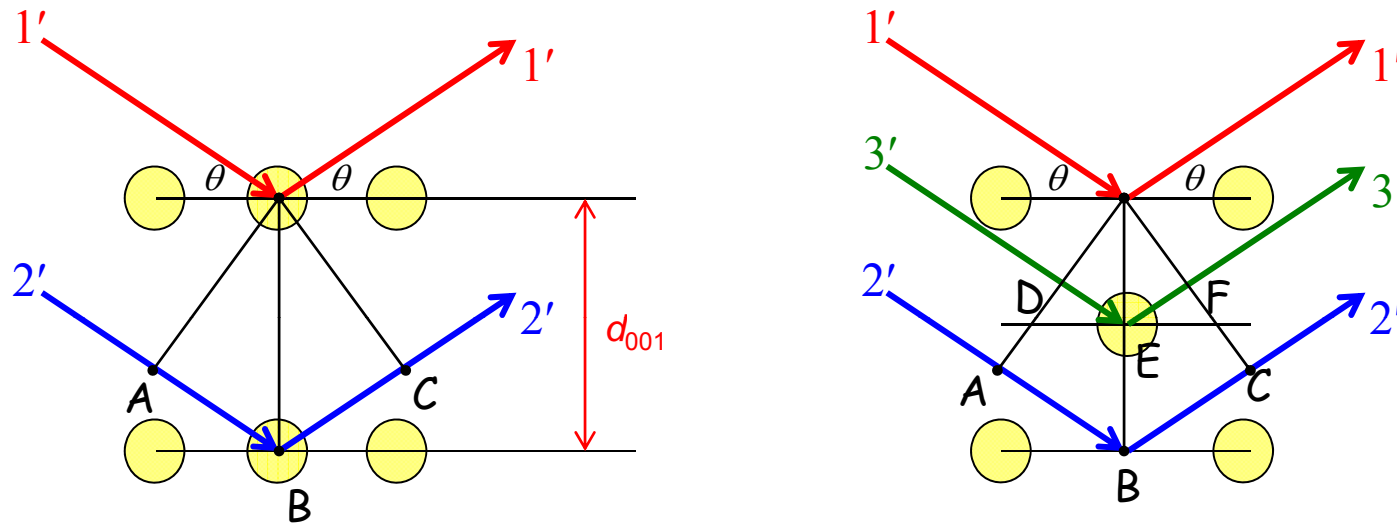


Consider the base-centered and body-centered orthorhombic unit cells drawn above.

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

[consider all orders]

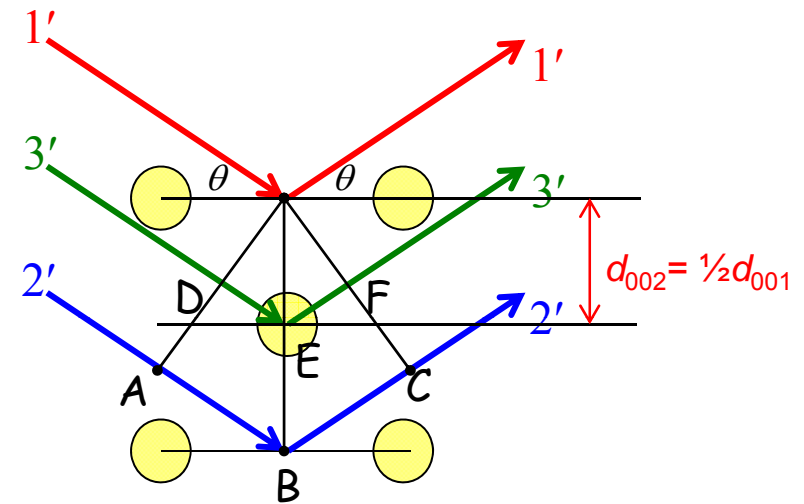
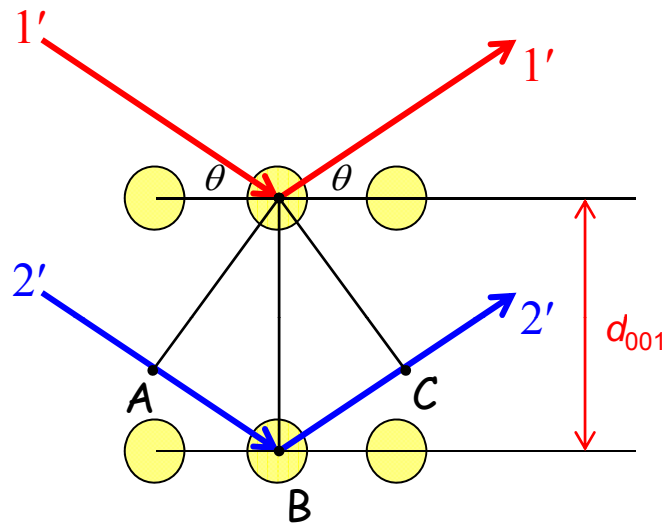
# Diffraction from (001)



## In Both Unit Cells

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

# Diffraction from (001)



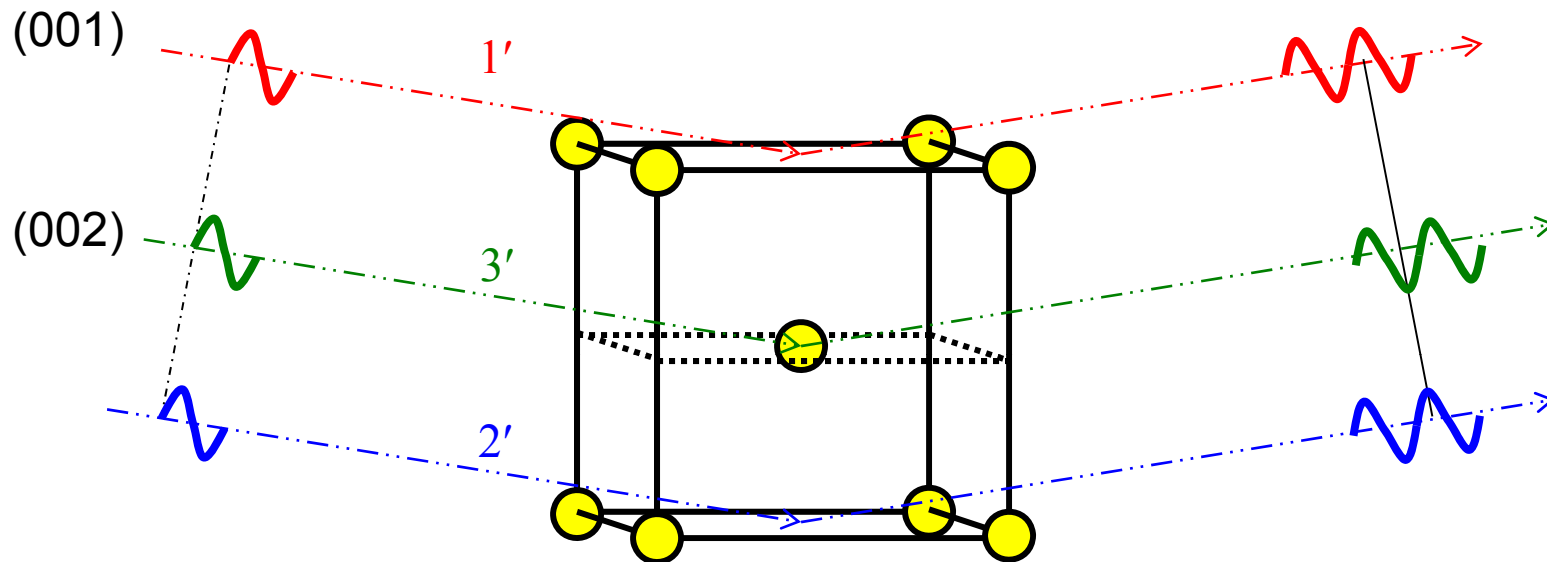
## In the Body Centered Unit Cell

The path difference between rays 1' and 3',  
 $\delta_{1'-3'} (i.e., DEF) = \frac{1}{2} \times \delta_{1'-2'} (i.e., \text{one wavelength})$

or

$$\delta_{1'-3'} = \frac{1}{2} \times \lambda (i.e., 180^\circ)$$

# 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.