

# Monday, April 20

## Last Time:

- Introduction to diffraction
- Bragg's Law and powder diffraction

## Readings:

- Chapter 23
- Solid State handout

## Today:

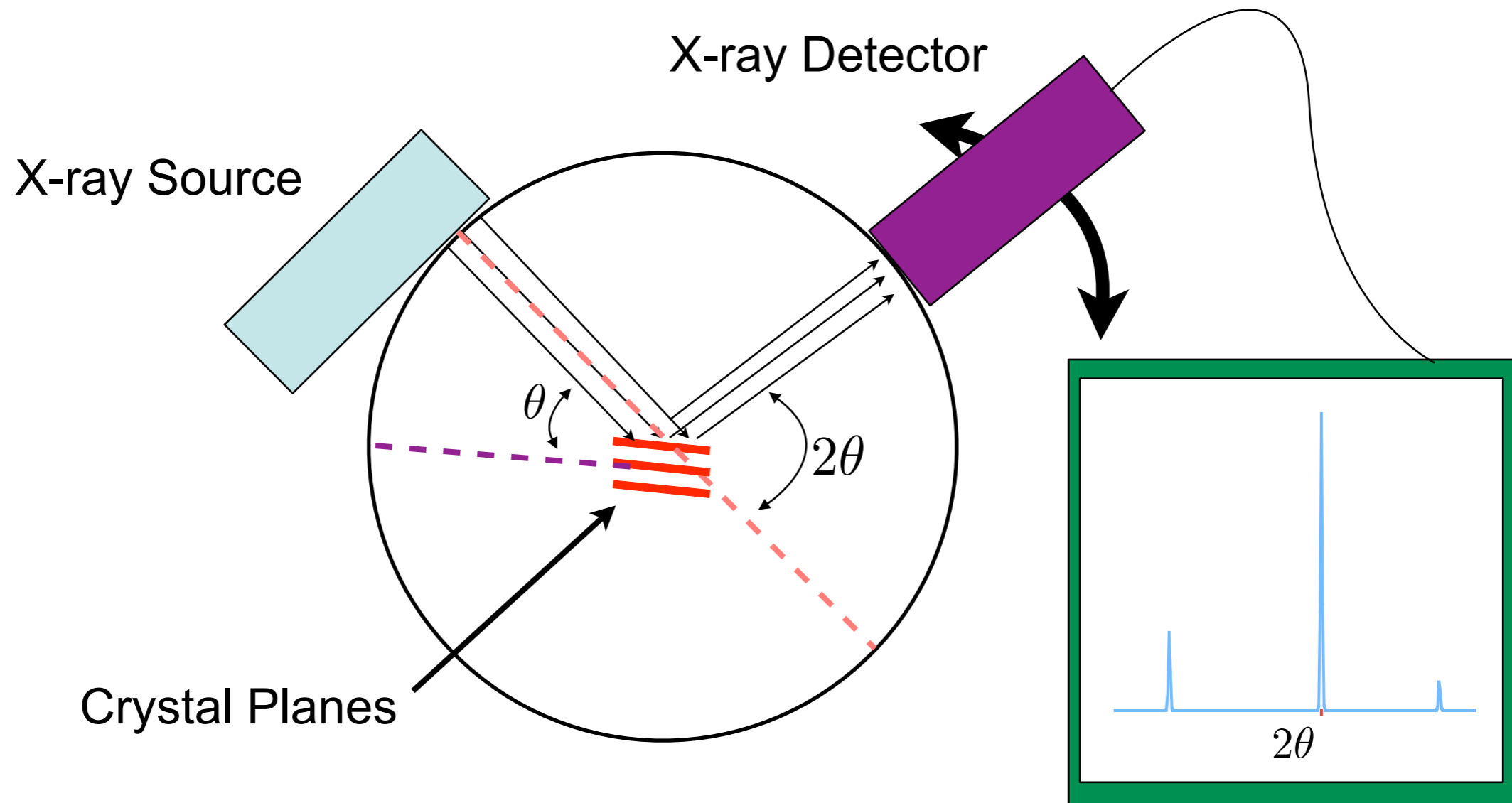
- Non-primitive structure
- Systematic absences and non-primitive structures
- More complex structures
- Course evaluations

## Handouts:

## Reminders:

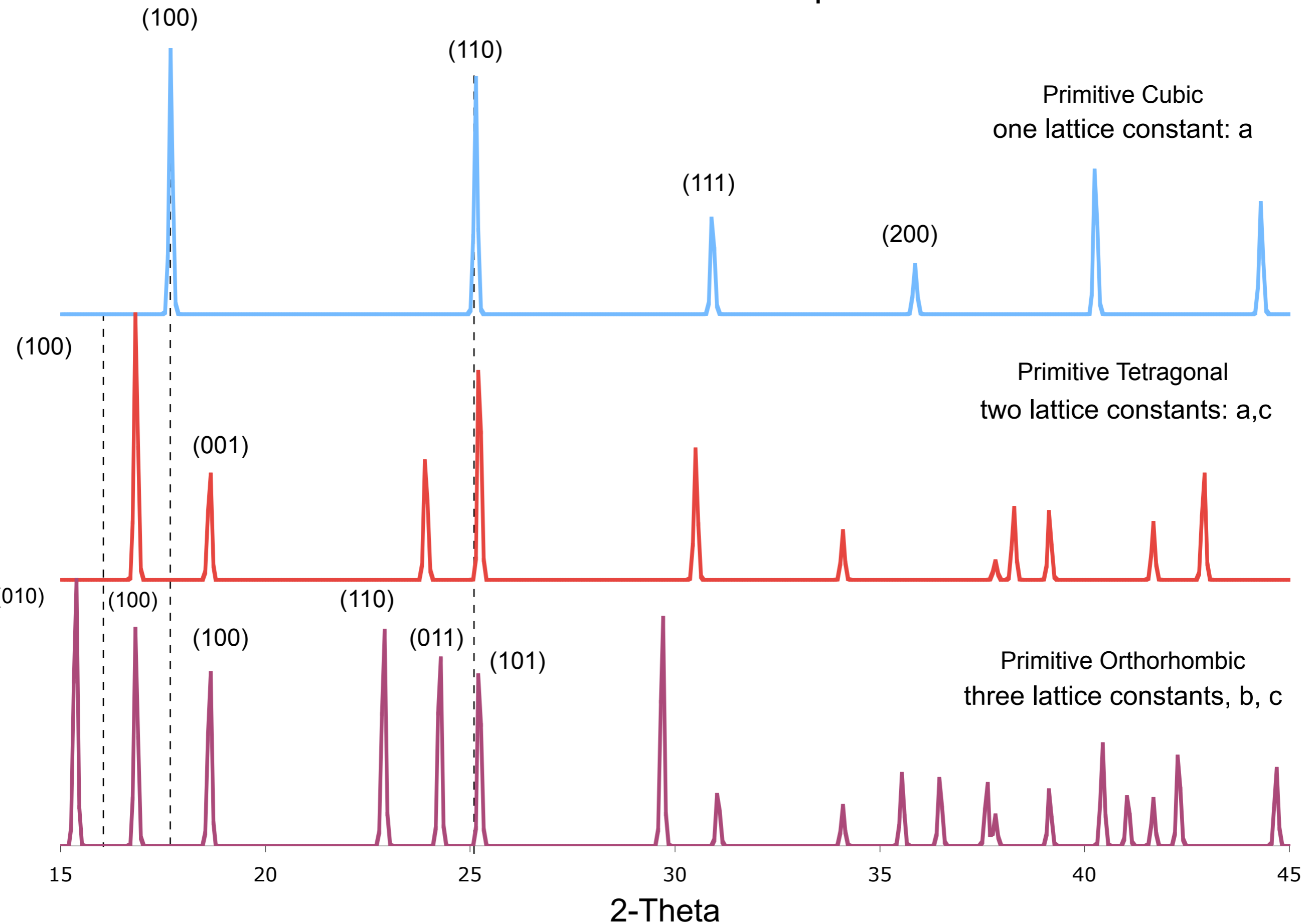
- Homework #9 for Wednesday
- Guest speaker Wednesday

# Typical powder x-ray diffraction geometry



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

# Primitive Cells - Diffraction patterns

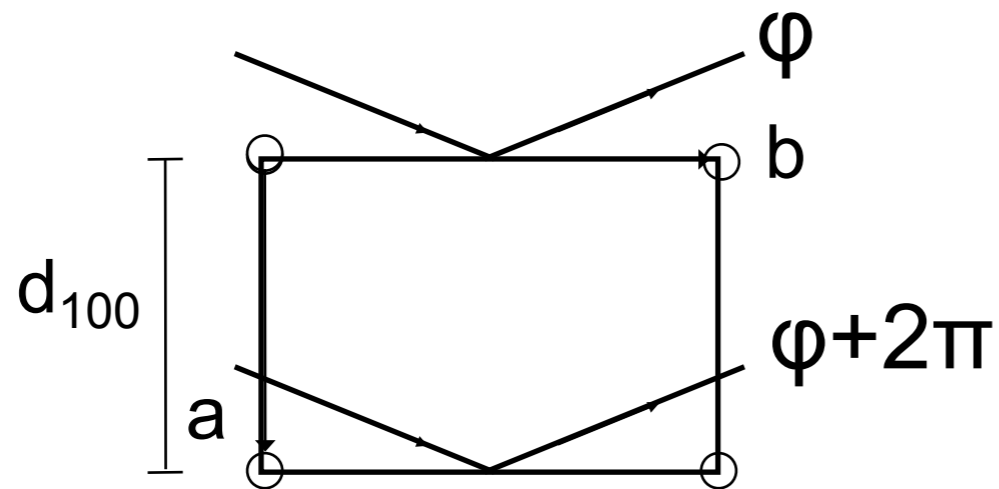


# Absent Reflections

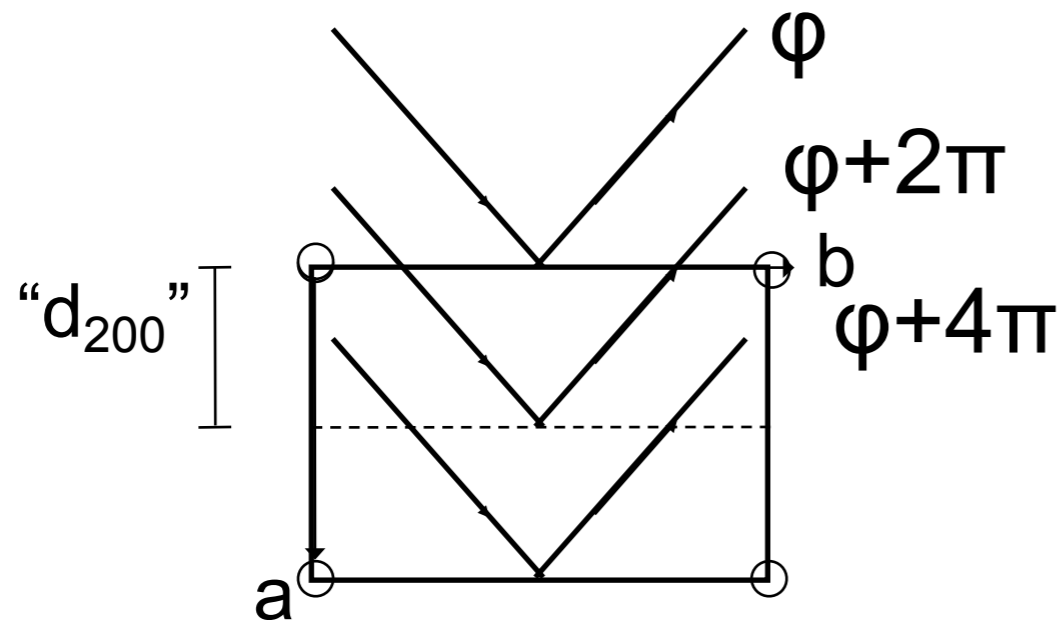
Due to Non-Primitive Lattice Type

Primitive  
No absences

(100)



(200)



[Note: First order from (200) =  
Second order from 100)]

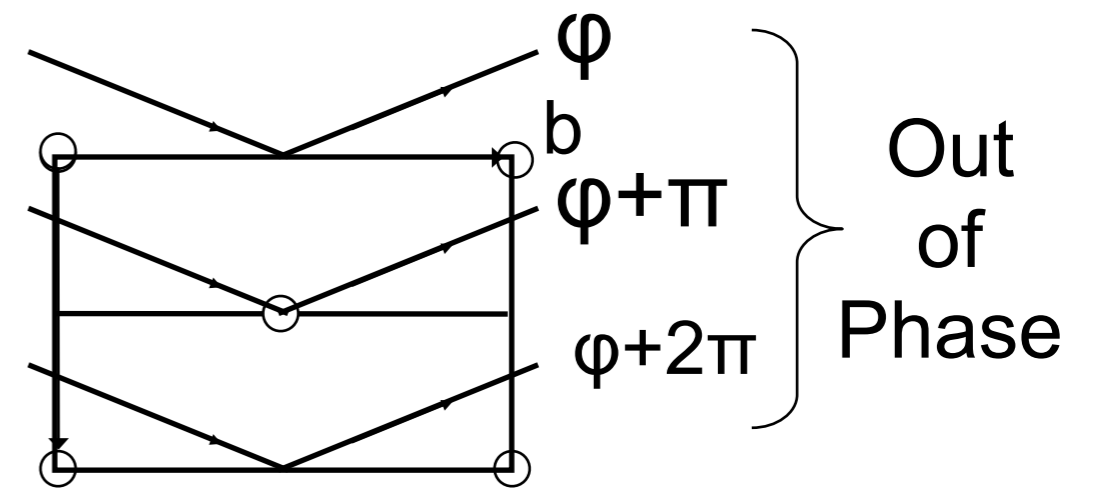
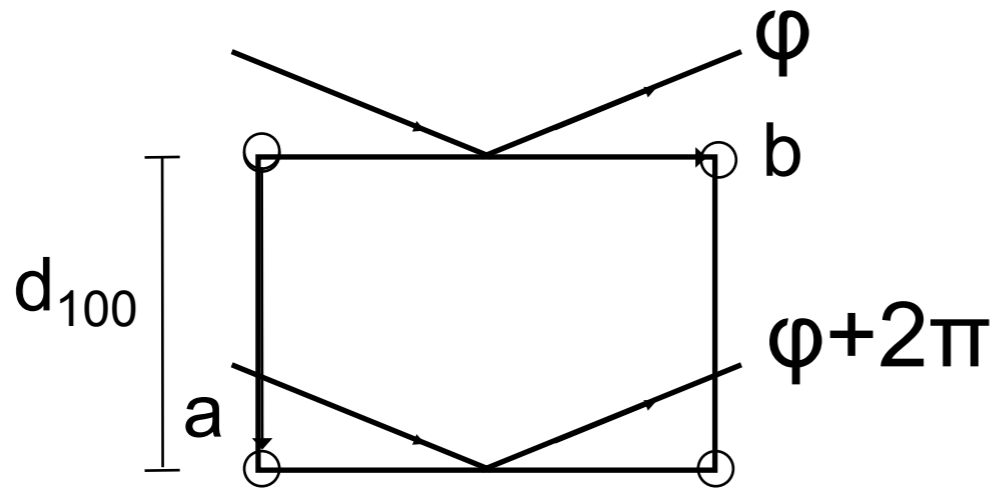
# Absent Reflections

Due to Non-Primitive Lattice Type

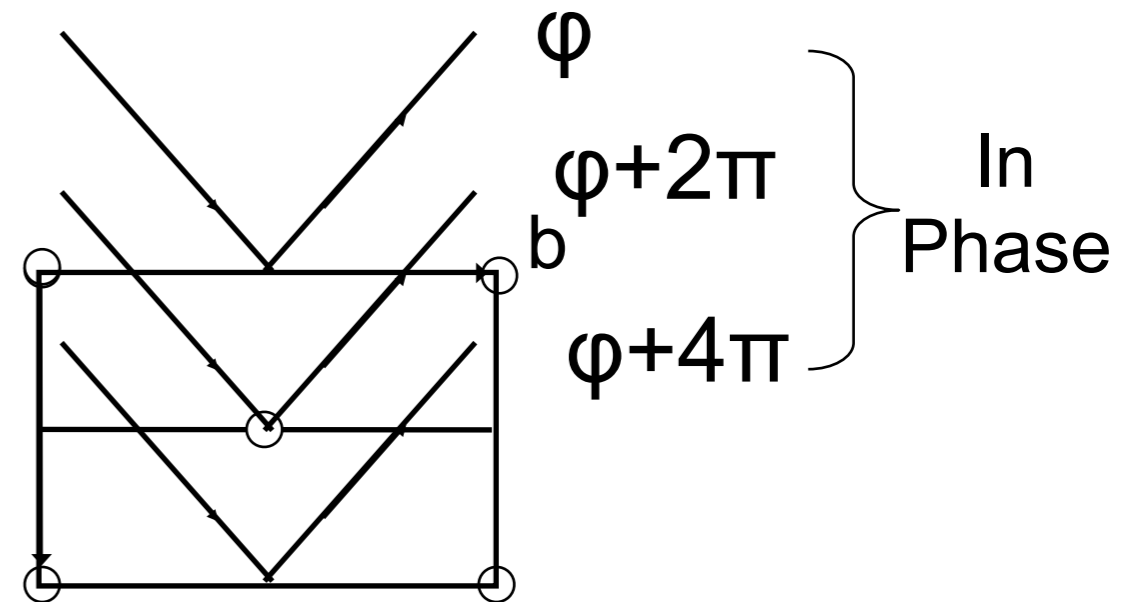
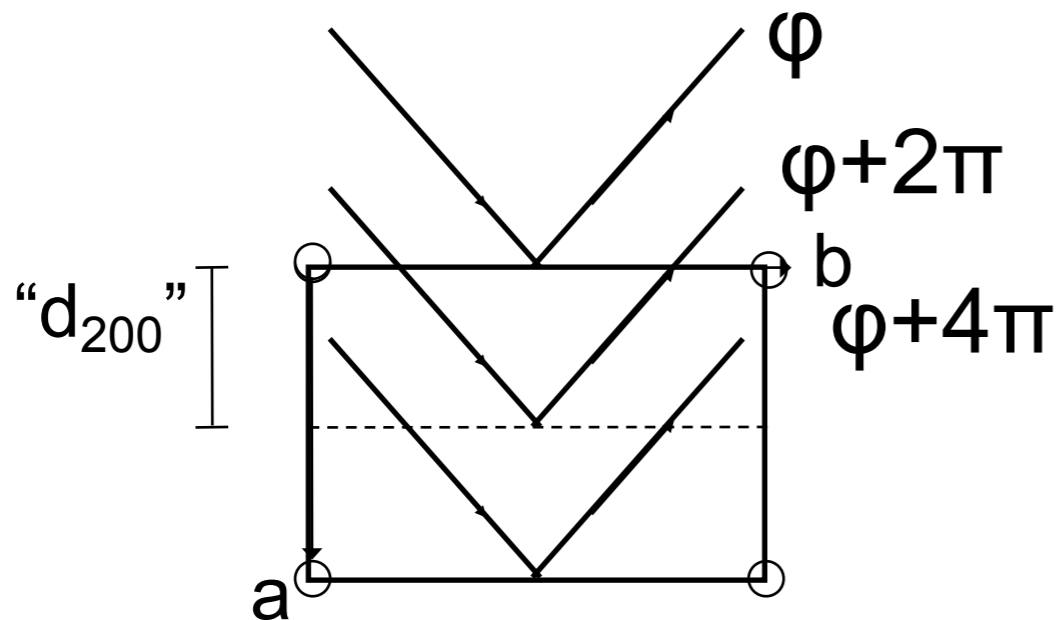
Primitive  
No absences

Side Centered  
 $h+k \neq 2n$  absent

(100)



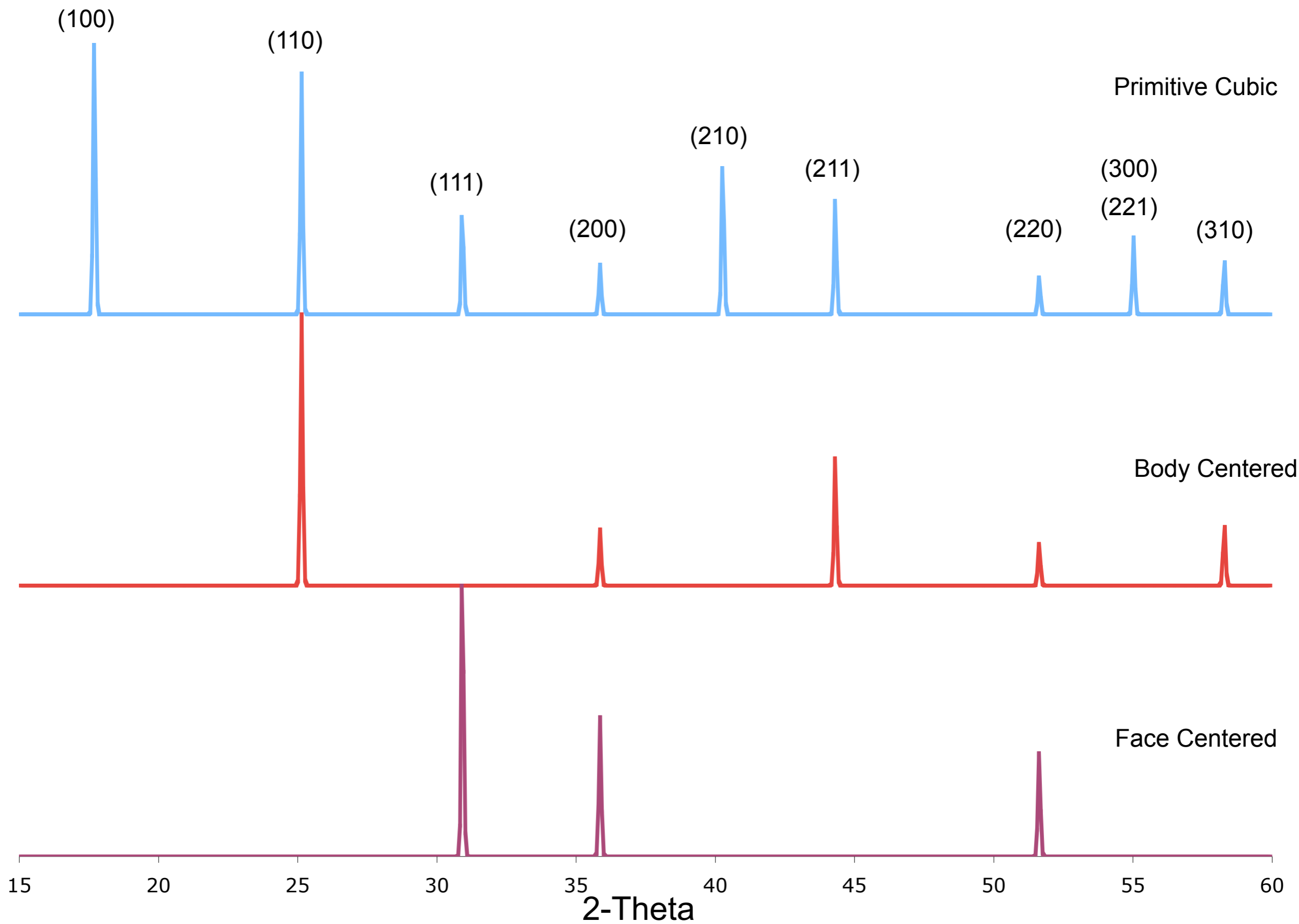
(200)



[Note: First order from (200) =  
Second order from 100)]

[Note: First order from (200)  
exists because of the side  
centered atom]

# Systematic Absences - Multiple Cells



# Five-step program for determining crystal structure

1. Start with  $2\theta$  values and generate a set of  $\sin^2 \theta$  values.
2. Normalize the  $\sin^2 \theta$  values by generating  $\frac{\sin^2 \theta_n}{\sin^2 \theta_1}$ .
3. Clear fractions from “normalized” column.
4. Speculate on the  $hkl$  values that, if expressed as  $h^2 + k^2 + l^2$  would generate the sequence of the “clear fractions” column.
5. Compute for each  $\theta$  the value of  $\frac{\sin^2 \theta}{h^2 + k^2 + l^2}$  on the basis of the assumed  $hkl$ . If each entry in this column is identical, then the entire process is validated.

2T	$\sin^2 T$ (1)	normalized (2)	clear fractions (3)	(hkl)? (4)	check (5)
44.48°	0.143	1.00	3	111	0.0477
51.83	0.191	1.34	4	200	0.0478
76.35	0.382	2.67	8	220	0.0478
92.90	0.525	3.67	11	311	0.0477
98.50	0.573	4.01	12	222	0.0478
121.87	0.764	5.34	16	400	0.0477
144.54	0.907	6.34	19	331	0.0477
155.51	0.955	6.68	20	420	0.0478

  
**FCC**