

Friday, April 24

Last Time:

- Non-primitive structures and diffraction
- Systematic absences

Today:

- FCC structures: systematic absences
- More than one atom type per unit cell?
- Chemical order

Readings:

- Chapter 23
- Solid State handout

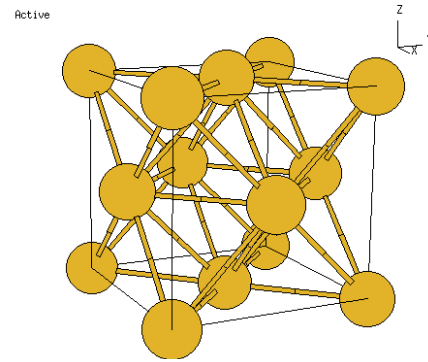
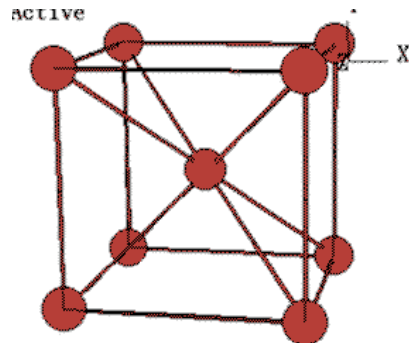
Handouts:

Reminders:

- Seminar speaker today: 11:30, B-105
“Mechanistic studies on the reactions of Chromium-complexed arenes”



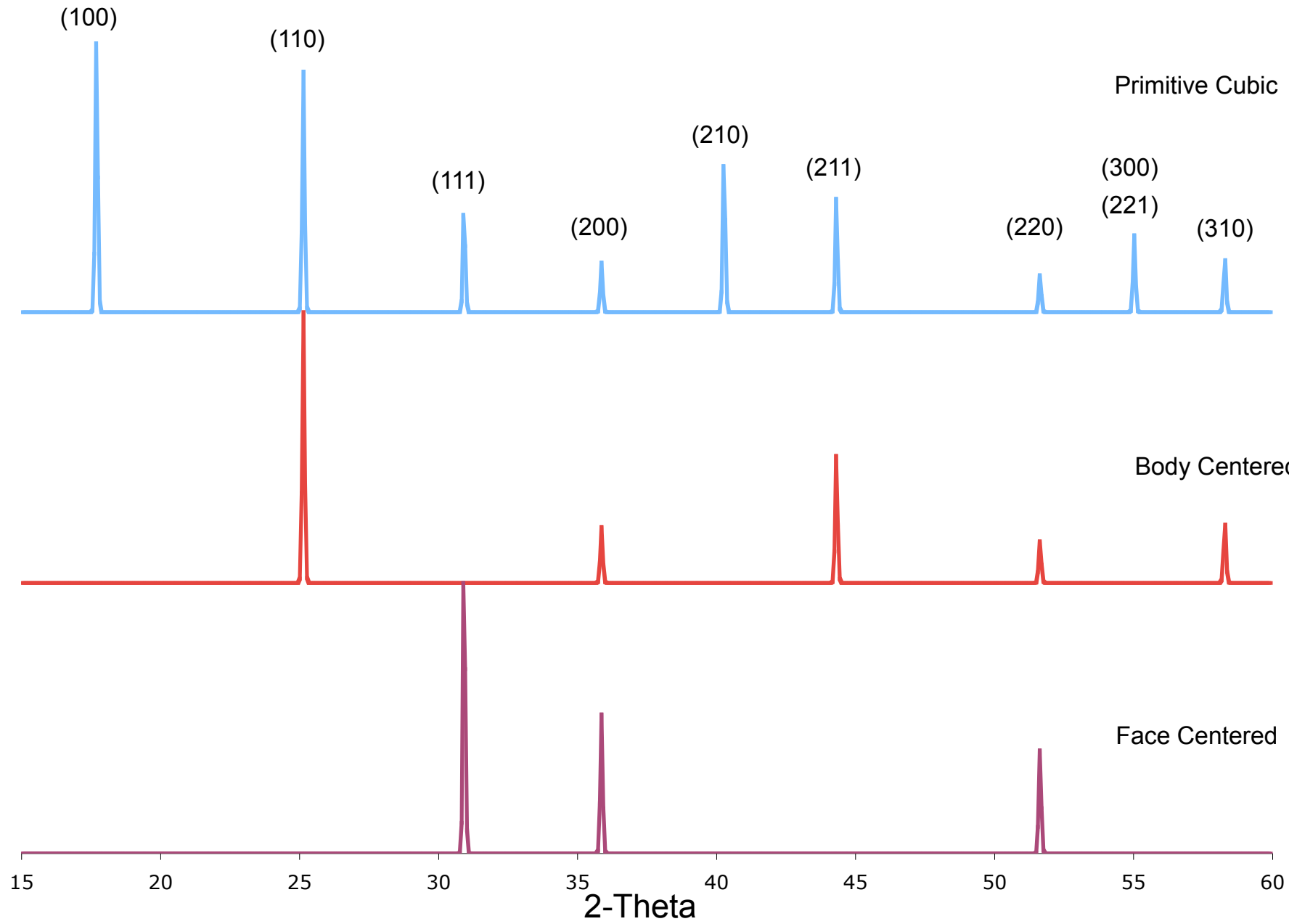
Structure Factor and Systematic Absences



$$F_{hkl} = \sum_{cell} f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

Primitive Cubic	BCC	FCC
All reflections allowed	$h + k + l = \text{even}, F \neq 0$ $h + k + l = \text{odd}, F = 0$	h, k, l all even or all odd, $F \neq 0$ h, k, l mixed even and odd, $F = 0$

Systematic Absences - Multiple Cells



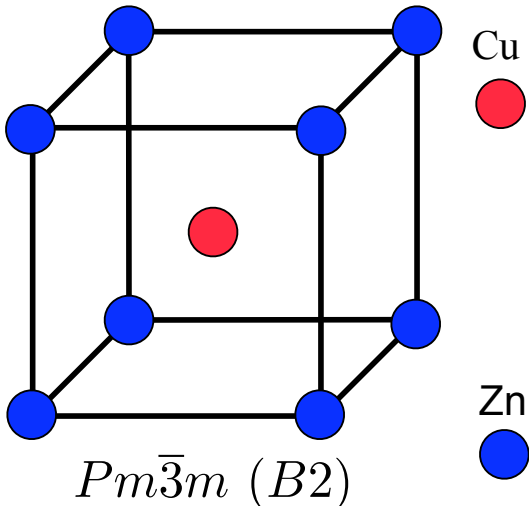
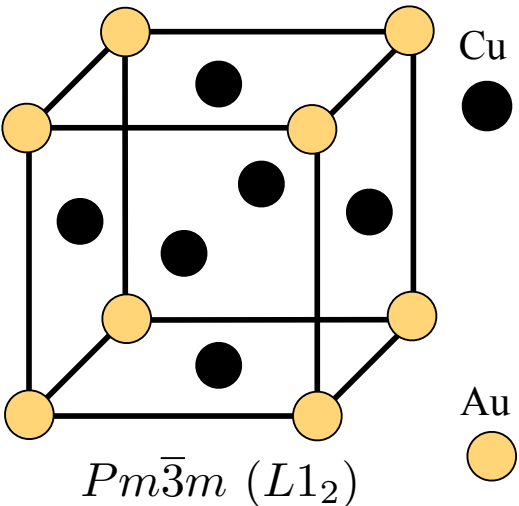
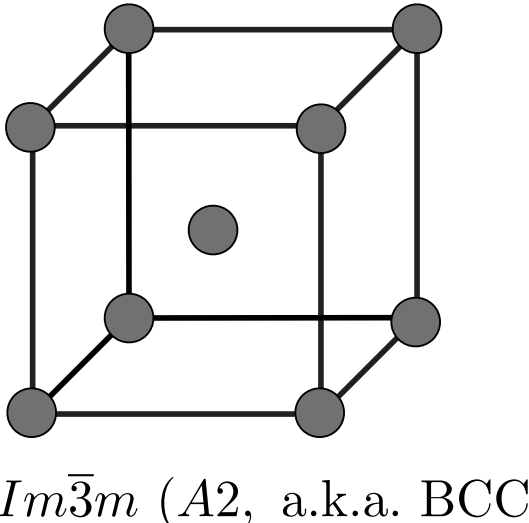
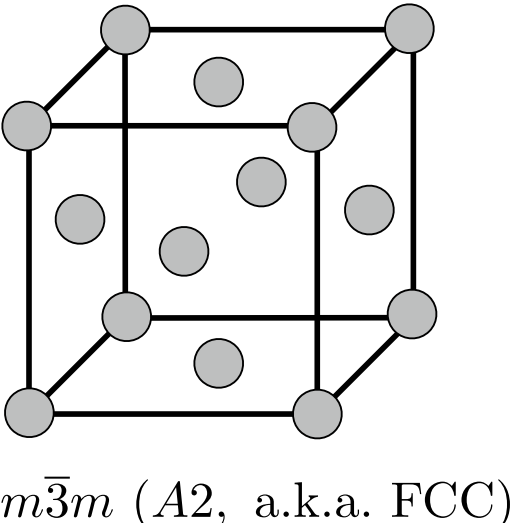
Five-step program for determining crystal structure

1. Start with 2θ 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 θ 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.

2 θ	$\sin^2\theta$ (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

Chemical Order

	CuZn (β -Brass)	Cu ₃ Au
Ordered	 <p>$Pm\bar{3}m$ ($B2$)</p>	 <p>$Pm\bar{3}m$ ($L1_2$)</p>
Disordered	 <p>$Im\bar{3}m$ ($A2$, a.k.a. BCC)</p>	 <p>$Fm\bar{3}m$ ($A2$, a.k.a. FCC)</p>

