

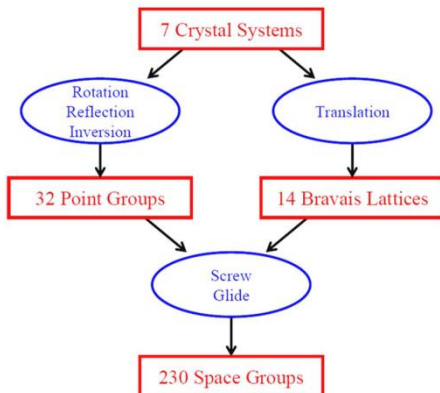


# Review Topics for Final (since Midterm)

Final is comprehensive but will be weighted more on material covered after midterm (~90%)

## 1. Crystallography ~ 35% test (classes 13-23)

1. Know the 7 crystal systems, 14 Bravais lattices, and their minimum symmetry requirements.
2. Crystal structure = Bravais lattice + **basis positions**
3. Take Bravais lattices step further → 10 2-D point groups (rotation and reflection) and 17 2-D plane groups (10 2-D point groups + 5 2-D Bravais lattices + glide).
4. Recognize any 2-D pattern and determine lattices + symmetry types (=plane group).
5. Know all symmetry operators and groups of operators and be able to recognize them in shapes/objects and more importantly crystal structures (in 3-D):



6. For 32 3-D point groups know their order (based on minimum symmetry requirements):

**Table 9.1.** Primary, secondary, and tertiary symmetry directions in each of the seven crystal systems. For the tetragonal system, the symbol  $\langle uvw \rangle$  refers to the fact that equivalent directions are obtained from permutations of the first two indices only.

| Crystal system | Primary $[uvw]$       | Secondary $[uvw]$       | Tertiary $[uvw]$        |
|----------------|-----------------------|-------------------------|-------------------------|
| Cubic          | $\langle 100 \rangle$ | $\langle 111 \rangle$   | $\langle 110 \rangle$   |
| Hexagonal      | $[00.1] = [0001]$     | $[10.0] = [2\bar{1}10]$ | $[12.0] = [01\bar{1}0]$ |
| Tetragonal     | $[001]$               | $\langle 100 \rangle$   | $\langle 110 \rangle$   |
| Orthorhombic   | $[100]$               | $[010]$                 | $[001]$                 |
| Trigonal       | $[111]$               | $[010]$                 | $[1\bar{1}0]$           |
| Monoclinic     | $[010]$               | —                       | —                       |
| Triclinic      | —                     | —                       | —                       |



# Review Topics for Final (since Midterm) (continued)

7. Point group symmetry can have a profound affect on physical properties of crystals → be familiar with the physical properties table and know Neumann's Law and see its relevance to tensor materials properties.
  8. Understand the group of symmetry operators involving microscopic translation → glide and screw
  9. For any of the 230 space groups be able to recognize its corresponding Bravais lattice and Point group.
  10. Be able to interpret the space group information given in the International Tables for Crystallography (number of basis positions, centering operations, Wyckoff notation, etc.) and apply it to crystal structures, as examples we went over  $\text{CrSi}_2$  and  $\text{TiAl}_3$  in class.
  11. To summarize crystallography, consult the “Review of Crystallography” slides given in Class 23 notes.
2. Diffraction ~ 55% test (classes 24-27)
1. Know Bragg's law and its physical meaning; concept of constructive vs. destructive interference
  2. Be familiar with interplanar ( $d_{hkl}$ ) spacings table for the 7 crystal systems and how it can be equated with Bragg's law
  3. Recognize why as crystal symmetry decreases, the number of XRD peaks observed increases
  4. Know the selection rules for cubic structures (with respect to primitive and non-primitive lattices)
  5. Understand why the arrangement of atoms within the unit cell is associated with the relative intensities of diffraction peaks
  6. Determine how unit cell distortions (symmetry) affect XRD patterns, peak splitting and change in d-spacings and  $2\theta$  values.
  7. Know the structure factor (F) and its physical meaning (equation tells us what reflections (hkl) to expect in a diffraction pattern from a given crystal structure with atoms located at positions u,v,w)



# Review Topics for Final (since Midterm) (continued)

8. Structure factor also permits us to calculate the intensity of any hkl reflection from a knowledge of the atomic positions.
9. Know the structure factor calculations for all the centering operations (I, F, A, B, C) – *we went over I in class and the others are in the handout.*
10. Determine whether a crystal structure is centric or non-centric, and once known its relation to Euler's formula for calculating the structure factor and intensity.
11. Understand and apply the 3 main factors that contribute to the diffraction intensity (F, p and LP)
12. Calculate x-ray intensities, we did Cu (FCC metal), TiO<sub>2</sub> (rutile), and ZnTe (zincblende) in class.
13. Know under what conditions the calculated intensities agree or disagree with powder diffraction files.
14. Be able to determine selection rules based on structure factors calculations.
15. Recognize from XRD if a material exhibits random orientation or preferred orientation (texture).



# Chapters to Review in DeGraef book

1<sup>st</sup> & 2<sup>nd</sup> editions: Chapters 2-5, 7-12, 14, 17, 22, 23