Materials 218/Chem277: Assignment 4

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This is a sample midterm exam.

1. The structure of a half-Heusler compound formed from Ti, Co, and Sb is described:
   Space group $F4\bar{3}m$ (No. 216) a = 5.888 Å.

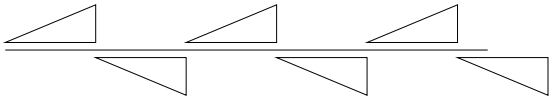
Atom	Wyckoff Position	x	y	z
Ti	4a	0	0	0
Co	4c	1/4	1/4	1/4
Sb	4b	1/2	1/2	1/2

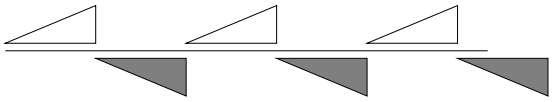
   Note: You should NOT require space group tables.

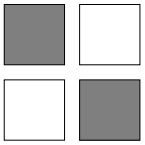
   (a) What is the formula of the compound ?
   (b) How many atoms of each kind are there in the unit cell ?
   (c) Sketch the various sections in the structure.
   (d) Describe the structure in terms of interpenetrating lattices.
   (e) How is the structure related to rock salt ?
   (f) How is the structure related to zinc blende ?
   (g) What is the coordination of Co in terms of Sb ?
   (h) What is the coordination of Ti in terms of Sb ?
   (i) Can you interchange the positions of Ti and Sb without changing the structure ?
   (j) What would the formula of the compound be for the same atom positions, perhaps different Wyckoff numbers, but in the space group $Fm\bar{3}m$ (the space group of NaCl and CaF_2) ?

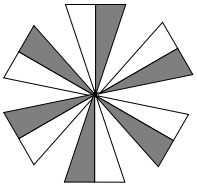
2. Sketch the cubic perovskite $BaZrO_3$ (Ba^{2+}, Zr^{4+}, O^{2+}) with Ba in the corners and Zr in the center of the cube. How many Ba and how many Zr are each O bonded to ? Verify that the rules of electrostatic bond valence are obeyed by considering all bonds coming to oxygen from the cations (remember its Ba^{2+}, Zr^{4+}, and O^{2-}).

3. The questions (a), (b), (c), and (d) correspond to the figures below:

   (a)
   

   (b)
   

   (c)
   

   (d)
   

(a) Identify the line group.

(b) Identify the line group, including color.

(c) Identify *all* the mirrors and *all* the rotations (normal symmetry and color symmetry).

(d) Identify *all* the mirrors and *all* the rotations (normal symmetry and color symmetry).

(e) Why can't a square lattice be centered (show a sketch) ?

(f) Can a square lattice with the symmetry $4mm$ support a dipole moment ? [A dipole moment means the centers of positive and negative charges in the unit cell do not coincide].

(g) What kind of operation (in 2D) is signified by $(0,0)+$ and $(\frac{1}{2},\frac{1}{2})+$?

(h) What kind of operation (in 3D) is signified by $(0,0,0)+$; $(0,\frac{1}{2},\frac{1}{2})+$; $(\frac{1}{2},0,\frac{1}{2})+$ and $(\frac{1}{2},\frac{1}{2},0)+$?

(i) True or false: In 2D systems, 3 and 6-fold symmetries are compatible with glide planes ?

(j) What new classes of symmetry operations are encountered on going from 1D and 2D, to 3D ? Sketch at least two.