Assignment 3

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Submit to Paul by Tuesday 10/26/2004.

Remember the in-class midterm on October 28

1. A certain perovskite ABO_3 is cubic with $a = 4.00$ Å. Plot the structure in sections and use this to demonstrate that:

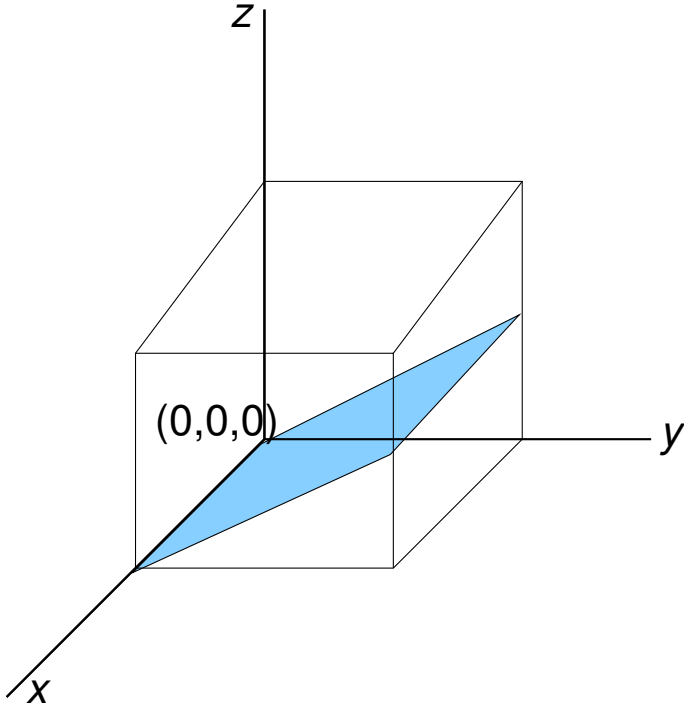
   (a) The A atom has 12 O nearest neighbors. What is the A-O distance ?

   (b) The B atom has 6 O neighbors. What is the B-O distance ?

   (c) What is the ratio of the A-O distance to the B-O distance ?

   (d) Demonstrate using a suitable sketch, that the section in the ABO_3 structure with A atoms and O is the same as any section of the rock-salt (NaCl) structure.

2. In the following figure, label the indicated Miller planes



3. Use the same coordinate system and cell as in the previous figure to sketch the following Miller planes and directions:

   (a) Planes: (110), $(\bar{1}10)$, $(\bar{1}11)$

   (b) Directions: [110], [210], [123]

4. The compound Na_2O has a cubic unit cell. O atoms (by themselves) form an fcc structure. The Na atoms sit in the following 8 positions:
   $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ $(\frac{3}{4}, \frac{1}{4}, \frac{1}{4})$ $(\frac{1}{4}, \frac{3}{4}, \frac{1}{4})$ $(\frac{3}{4}, \frac{3}{4}, \frac{1}{4})$ $(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $(\frac{3}{4}, \frac{1}{4}, \frac{3}{4})$ $(\frac{1}{4}, \frac{3}{4}, \frac{3}{4})$ $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$
   Sketch the structure as sections. Do you recognize it ? How many O neighbors do Na have and how many Na neighbors do O have ?

5. The (h, k, l) Miller planes in a tetragonal compound with $a = 4.00$ Å and $c = 6.00$ Å give rise to a series of reflections in the X-ray diffraction pattern. Using the relation (for tetragonal cells):

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

calculate the θ values (in degrees) for which X-ray reflections will be observed corresponding to the following planes: (100), (110), (200), (222), (004). Use $\lambda = 1.5$ Å, and the Bragg law: $2d_{hkl} \sin\theta = \lambda$.

6. What would the formula for the tetragonal cell:

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

look like for a cubic cell ? For what kinds of cells (crystal systems) would the following formula *not* hold and why:

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$