MSAE E4100 Crystallography
Fall 2016
Barmak

Homework 4 - Update
Due Thursday October 6, 2016
100 points

Reading assignment: Chapters 1-5 Burns and Glazer. Chapters 4-7 De Graef and McHenry, or any other book that covers the topics covered in these chapter. Lectures 1-5, Lecture 10 in its entirety.

<u>For questions that ask you to use the RPC set, you will receive no credit if you do not do so.</u>

1. [8+2=10 points]
    a. Use the flow chart (logic tree) on slide 63 of Lecture 4 to determine the point groups for the eclipsed and staggered configurations of the methane molecule, C_2H_6 (See HW 1). List each question sequentially and give the answer. So for example: 1. Is the molecule linear? N.
    b. List the point groups using both the Schoenflies and the ITA notations.

2. [4 points] Find the cross product of the pair of directions $\left[10\bar{3}\right]$ and $\left[511\right]$ in the monoclinic system.

3. [6 points] If a vector has components (2,1,3) with respect to the basis vectors of the direct space lattice with lattice parameters {0.500,0.500,0.816,90,90,120}, then what are the components of that vector with respect to the reciprocal basis vectors?

4. [10 points] Given are two zones described by the sets of planes of the type $\left\{h\bar{h}l\right\}$ and $\left\{h0h\right\}$. What is the normal to the plane formed by the two corresponding zone axes?

5. [5 points] Use your RPC set to draw a stereographic projection to show that 3[001] and 2[010] lead to the creation of 2[100] and 2[110]?

6. [5+3+8×4=40 points] Determine the coordinate transformation matrix α_{ij} that expresses the basis vectors of the primitive unit cell of the body centered cubic lattice in terms of those of the conventional unit cell of this lattice. If we denote quantities in the cubic reference frame by a subscript *c*, and quantities in the primitive reference frame by a subscript *p*, then answer the following questions (a)–(i).

Use the following basis vectors (rather than choosing your own so that we all start from the same point):

$$\mathbf{a}_{1p} = \frac{1}{2}\left(-\mathbf{a}_{1c} + \mathbf{a}_{2c} - \mathbf{a}_{3c}\right)$$

$$\mathbf{a}_{2p} = \frac{1}{2}\left(-\mathbf{a}_{1c} - \mathbf{a}_{2c} + \mathbf{a}_{3c}\right)$$

$$\mathbf{a}_{3p} = \frac{1}{2}\left(\mathbf{a}_{1c} + \mathbf{a}_{2c} + \mathbf{a}_{3c}\right)$$

a. Draw several body centered cubic unit cells. Then draw the primitive (rhombohedral) basis vectors given above on the same drawing.
b. Give the coordinate transformation matrix $\boldsymbol{\alpha}_{ij}$ that expresses the basis vectors of the primitive unit cell of the body centered cubic lattice in terms of those of the conventional unit cell of this lattice.
c. Determine the inverse transformation matrix.
d. What are the c components of the position vector $\left(\frac{1}{2},\frac{1}{3},\frac{2}{5}\right)_p$?
e. What are the *p* components of the normal to the plane $\left(\bar{5}23\right)_c$?
f. Write down the c zone equation for the $[311]_p$ zone axis.
g. What are the *p* components of the direction vectors $[110]_c$?
h. What are the *c* components of the normal to the plane $(102)_p$?
i. What are the *c* components of the direction vectors $\left[\bar{1}01\right]_p$?
j. What is the volume of the *p* unit cell?

7. [2+2+6+2+5+8=25 points] Use your RPC set.
   a. Make a schematic drawing of the water molecule with the molecule placed in the plane of the page.
   b. Make a schematic drawing of the molecule looking along the line that bisects the OH bonds. Draw the molecule with the bonds along the horizontal axis, which we will term the **b**-axis, with the positive direction pointing to the right.
   c. What are the symmetry operations of the H_2O molecule? Choose the axis of projection in (b) as your **c**-axis. The **b**-axis was given in (b). Take the **a**-axis pointing down on the page. Give the symmetry operations in columns and list both the ITA notation and the Schoenflies notation.
   d. What is the point group of the water molecule? Give both the ITA and Schoenflies designations.
   e. Use the symmetry operators to create the symmetry equivalent points on a stereographic projection for this point group. Give the symbols for the operators.
   f. Write the "multiplication table" for the symmetry operators (Note that these symmetry operators form the point group). To do this, make a table in which the columns are each of the symmetry operators including the symmetry axis. The first column is the identity operator, 1, and each of the rows are also the symmetry operators, with the first row also as 1. The entries in the table are the symmetry operators obtained by applying the symmetry operator listed in the column (first) followed by the symmetry operator listed in the row. The stereographic projection will aid you greatly in filling the entries in this table.