**MSAE E4100 Crystallography**
**Fall 2016**
**Barmak**

**Homework 3**
**Due Thursday September 29, 2016**
**100 points**

Reading assignment: Chapters 1-4 Burns and Glazer. Chapters 4-6 De Graef and McHenry, or any other book that covers the topics covered in these chapter. Lectures 1-4, Lecture 10 slides 1-64.

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

1. [2+2+4=8 points] The diamond cubic structure is a crystal structure adopted by C and many semiconducting materials such as Si, Ge, etc. The diamond structure has the cF Bravaid lattice with C atoms at (0,0,0) and (1/4,1/4,1/4), the diamond site. There are 8 atoms per unit cell in the structure and all atomic positions are generated from these given two by the centering vectors of the cF Bravais lattice. All the C atoms in the structure are 4-fold tetrahedrally coordinated by other C atoms.
    a. Express the direction of a bond between a C atom at the origin and the diamond site. Briefly explain how you arrived at the answer.
    b. Express the direction of a bond between a C atom at the origin and the C-face center. Briefly explain how you arrived at the answer.
    c. Use the metric tensor to calculate the bond angle between the two previous bonds.

2. [10 points] Graphite is an important solid lubricant and catalyst, in addition to being used as pencil lead in pencils that you should be using in doing your assignments for this class! Its structure consists of hexagonal networks of C atoms stacked along the **c**-axis; atoms in one layer are located above the center of the hexagons in the surrounding layers. Graphite has the lattice constants: {0.246,0.246,0.67, 90,90,120} (with a and c in nm).
    a. Determine the reciprocal metric tensor for graphite.
    b. Determine the angle between (111) and (100) planes for graphite using the reciprocal metric tensor.

3. [6×4=24 points] Consider a monoclinic lattice unit cell with lattice parameters {0.35,0.50, 0.44,90,105,90} given for the second setting.
    a. Determine the reciprocal metric tensor for this lattice. Note that the specific tensor given in the slide in Lecture 10 is for the second setting. The general tensor would apply to either setting.
    b. What is the distance between (120) planes?
    c. What is the angle between c* and the (310) plane normal?
    d. What is the angle between the (111) and $(\bar{1}11)$ planes?
    e. What is the volume of the direct space unit cell?
    f. What is the volume of the reciprocal space unit cell?

4. {8+3+3=14 points] Benzene, $C_6H_6$, is a molecular hydrocarbon (See Chapter 1 of Burns and Glazer). Benzene is a liquid at standard atmospheric pressure and temperature. The lowest pressure allotrope of solid benzene crystallizes at 0.7 kbar ($10^5$ bar = 1 atm) at room temperature and is orthorhombic with four formula units per unit cell. One formula unit is the unit given by the chemical formula, here $C_6H_6$. Given X-ray diffraction determined literature values for spacing between (200), (020) and (111) planes of 0.372, 0.478 and 0.448 nm, respectively, determine the following:
    a. The values of the a, b and c lattice constants.
    b. The volume of the unit cell.
    c. The density of this allotrope of solid benzene. Take the atomic weights of C and H as 12.0107 and 1.00794 g/mol, respectively.

5. [4+4+3+3=14 points] Use your RPC set to make accurate drawings for this question.
    a. Draw a 2-dimensional hexagonal lattice with a = 3 cm. Make your drawing a 4×4 set of unit cells, i.e., a total of 16 unit cells. Place the origin (0,0,0) at the centermost point of your drawing. Use solid lines for these unit cells.
    b. For the point at the origin, draw the Wigner-Seitz cell using dashed lines.
    c. Compute the ratio of the area of this cell to the area of the unit cell of the lattice.
    d. Compute the ratio of the area of the largest circle that can be contained inside this Wigner-Seitz cell to unit cell area of the hexagonal lattice.

6. [6+4=10 points] Use your RPC set to make an accurate drawing.
    a. Show that a C-centered (base centered) hexagonal lattice results in the orthorhombic crystal system. Draw the **c**-axis projection of a 2×2 set of unit cells to assist you in your demonstration. Use a value of a = 3 cm for your drawing. Put the origin at the centermost point of the drawing.
    b. What are the lattice parameters of the orthorhombic unit cell in terms of the original hexagonal lattice parameters?

7. [20 points] Use your RPC set to make an accurate drawing.
    a. Draw the [001] projection of simple orthorhombic direct space lattice, assuming that a = 2b and c = 3a. Make the drawing to scale. Take a = 35 mm and draw a 2×4 set of unit cells.
    b. Draw the [001]* projection of the reciprocal lattice (with *h* and *k* ranging from -2 to 2) of the simple orthorhombic direct lattice in part (a). Take a*=8.5 mm.
    c. Indicate the reciprocal lattice basis vectors and the unit cell of this reciprocal lattice.
    d. What is the volume of the reciprocal lattice unit cell? How is it related to the unit cell volume of the direct lattice?
    e. What happens to the volume of this reciprocal lattice when the direct lattice unit cell expands so that b remains the same, but a = 4b?

**Metric Tensors**

$$g_{\text{triclinic}} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ba\cos\gamma & b^2 & bc\cos\alpha \\ ca\cos\beta & cb\cos\alpha & c^2 \end{pmatrix}$$

$$g_{\text{monoclinic}} = \begin{pmatrix} a^2 & 0 & ac\cos\beta \\ 0 & b^2 & 0 \\ ca\cos\beta & 0 & c^2 \end{pmatrix}$$

$$g_{\text{orthorhombic}} = \begin{pmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}$$

$$g_{\text{tetragonal}} = \begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}$$

$$g_{\text{hexagonal}} = \begin{pmatrix} a^2 & -a^2/2 & 0 \\ -a^2/2 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}$$

$$g_{\text{rhombohedral}} = \begin{pmatrix} a^2 & a^2\cos\alpha & a^2\cos\alpha \\ a^2\cos\alpha & a^2 & a^2\cos\alpha \\ a^2\cos\alpha & a^2\cos\alpha & a^2 \end{pmatrix}$$

$$g_{\text{cubic}} = \begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & a^2 \end{pmatrix}$$

**Reciprocal Metric Tensor**

$$g^*_{\text{triclinic}} = \frac{1}{V^2}\begin{pmatrix} b^2c^2\sin^2\alpha & abc^2F(\alpha,\beta,\gamma) & ab^2cF(\gamma,\alpha,\beta) \\ abc^2F(\alpha,\beta,\gamma) & a^2c^2\sin^2\beta & a^2bcF(\beta,\gamma,\alpha) \\ ab^2cF(\gamma,\alpha,\beta) & a^2bcF(\beta,\gamma,\alpha) & a^2b^2\sin^2\gamma \end{pmatrix}$$

$$F(\alpha,\beta,\gamma) = \cos\alpha\cos\beta - \cos\gamma$$

*and*

$$V^2 = a^2b^2c^2\left(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma\right)$$

$$g^*_{\text{monoclinic}} = \begin{pmatrix} \frac{1}{a^2\sin^2\beta} & 0 & -\frac{\cos\beta}{ac\sin^2\beta} \\ 0 & \frac{1}{b^2} & 0 \\ -\frac{\cos\beta}{ac\sin^2\beta} & 0 & \frac{1}{c^2\sin^2\beta} \end{pmatrix}$$

$$g^*_{\text{orthorhombic}} = \begin{pmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{b^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$$

$$g^*_{\text{tetragonal}} = \begin{pmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{a^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$$

$$g^*_{\text{hexagonal}} = \begin{pmatrix} \frac{4}{3a^2} & \frac{2}{3a^2} & 0 \\ \frac{2}{3a^2} & \frac{4}{3a^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$$

$$g^*_{\text{rhombohedral}} = \frac{1}{W^2}\begin{pmatrix} 1+\cos\alpha & -\cos\alpha & -\cos\alpha \\ -\cos\alpha & 1+\cos\alpha & -\cos\alpha \\ -\cos\alpha & -\cos\alpha & 1+\cos\alpha \end{pmatrix}$$

$$W^2 = a^2\left(1+\cos\alpha-2\cos^2\alpha\right)$$

$$g^*_{\text{cubic}} = \begin{pmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{a^2} & 0 \\ 0 & 0 & \frac{1}{a^2} \end{pmatrix}$$

It can be shown that the reciprocal metric tensor is the inverses of the direct metric tensor. It can also be shown that the volume of the unit cell is the square root of the determinant of the metric tensor. It can further be shown that the volume of the unit cell in reciprocal space is the reciprocal of the volume of the unit cell in direct space.