MSE 102, Fall 2007 Midterm #1

Write your name here: _____

Instructions:

- Answer all questions to the best of your abilities. Be sure to write legibly and state your answers clearly.
- The point values for each question are indicated.
- You are not allowed to use notes, friends, phones, consultants, employees, etc.
- There are a total of 100 points.
- Feel free to ask questions, but only for clarification purposes.

Good luck. I sincerely hope you all do really well.

-Prof. Chrzan

1) A 2-D crystal has an atomic scale structure described by the symmetry group *p4mm* (see the attached entry from the International Tables for Crystallography). The lattice parameter (i.e. the length of the vector **a**) is equal to 2 Å. There are Si atoms at Wyckoff position(s) *a*, and C atoms at Wyckoff position(s) *c*.

Carry out the following instructions:

1. (8 points) On the attached graph paper, plot the positions of the lattice points with an ×. Plot all of the lattice points that appear in the range of the plot.

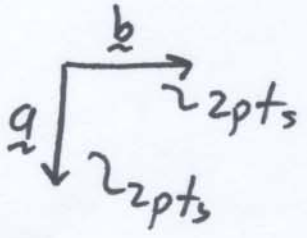
2. (8 points) Identify a set of primitive lattice vectors for the crystal. Write their coordinates here (in terms of $\mathbf{e}_x$ and $\mathbf{e}_y$) and draw them on your plot of the lattice.

3. (8 points) Give the basis vectors for the atoms. Label the *j*th basis vector of the Si atoms $\boldsymbol{\tau}_j^{Si}$, and the *j*th basis vector of the C atoms $\boldsymbol{\tau}_j^{C}$. Express the basis vectors in terms of your primitive lattice vectors defined in part 2 of this problem. How many atoms of each type does a unit cell contain?

1.1 a) each x is worth 1pt.

1.2 b) $\underline{b} = (2\underline{e}_x, 0)\,\text{Å}$ 2pts

$\underline{a} = (0, -2\underline{e}_y)\,\text{Å}$ 2pts



1.3) $\underline{\tau}_0^{Si} = 0\underline{a} + 0\underline{b}$ 2pts

$\underline{\tau}_1^{C} = \frac{1}{2}\underline{a} + 0\underline{b}$ 2pts

$\underline{\tau}_2^{C} = 0\underline{a} + \frac{1}{2}\underline{b}$ 2pts

Si → a sites
C → c sites

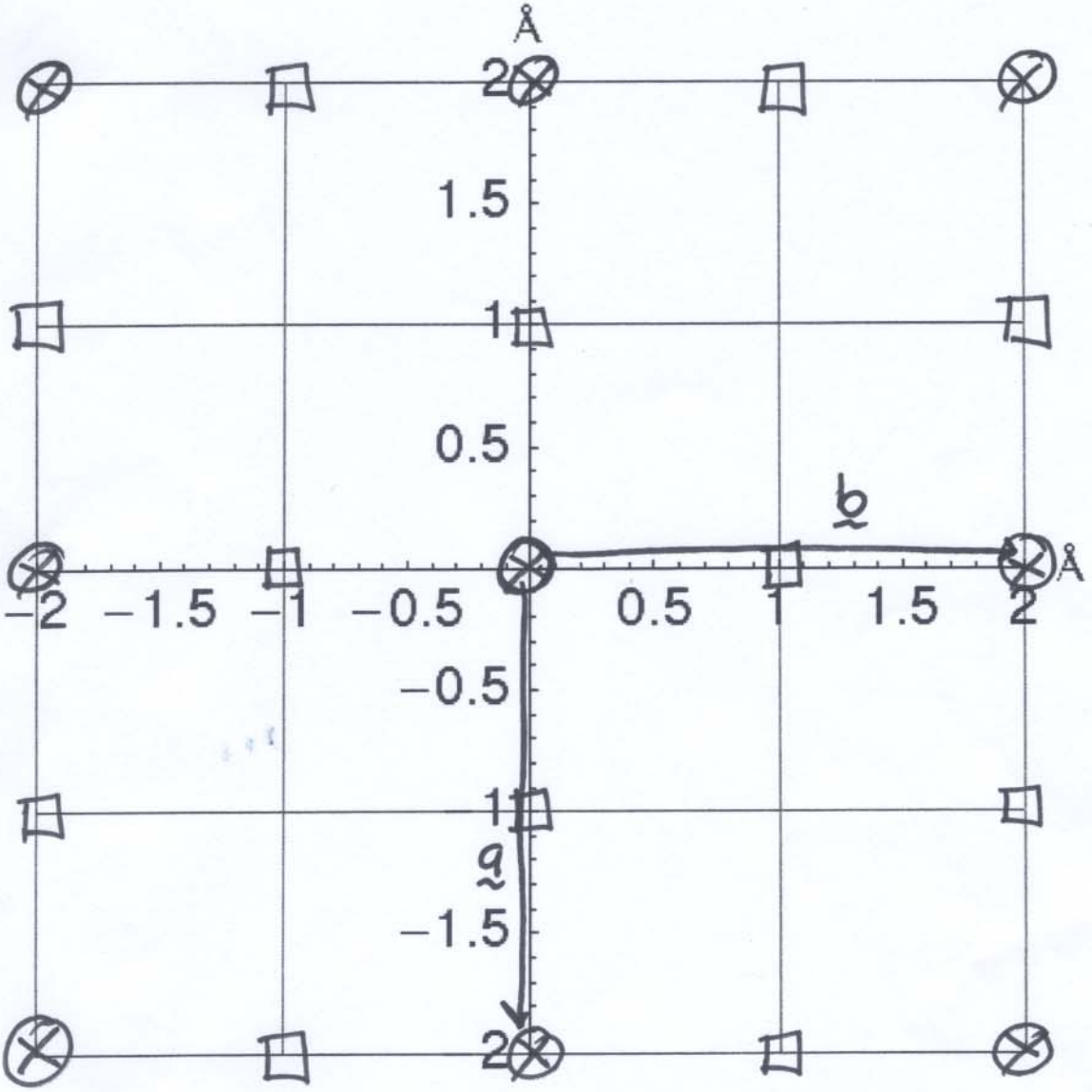
1 Si atom 1pt

2 C atom 1pt

1.4) The Si atom sits at 0,0 which is a lattice point which means that a Si atom has to occupy each lattice site.

just look at the single unit cell.

1pt each


Å
2
1.5
1
0.5
−2
−1.5
−1
−0.5
0.5
1
1.5
2
Å
−0.5
1
−1.5
2
b
q

1.5) $\underset{\sim}{a}^* \cdot \underset{\sim}{a} = 2\pi \qquad \underset{\sim}{a}^* \cdot \underset{\sim}{b} = 0$

$\underset{\sim}{b}^* \cdot \underset{\sim}{a} = 0 \qquad \underset{\sim}{b}^* \cdot \underset{\sim}{b} = 2\pi$

$\underset{\sim}{a}^* \cdot \underset{\sim}{a} = a_x^* a_x + a_y^* a_y = 2\pi$

$a_y^* a_y = 2\pi$

$a_y^* = \frac{2\pi}{a} = \pi \underline{e}_y$

$\underset{\sim}{b}^* \cdot \underset{\sim}{b} = b_x^* b_x + b_y^* b_y = 2\pi$

$b_x^* = \frac{2\pi}{b} = \pi \underline{e}_x$

The lattice vectors are perpendicular ∴ the other two eqns lead to 0s.

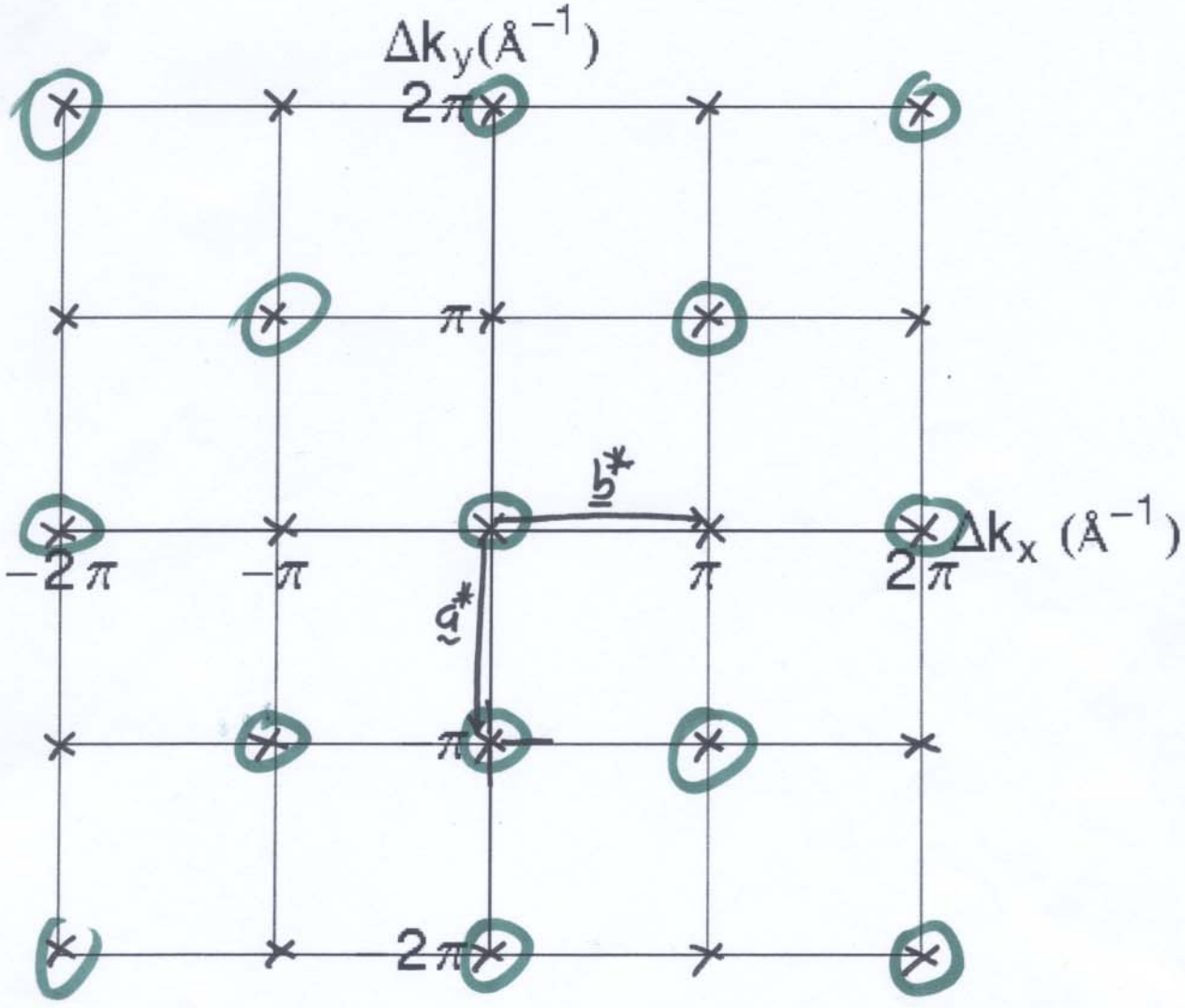
$\underset{\sim}{a}^* = 0\underline{e}_x - \pi \underline{e}_y$

$\underset{\sim}{b}^* = \pi \underline{e}_y + 0\underline{e}_y$

4. (8 points) On the same plot as that for part one, plot the positions of the Si atoms with an open circle and plot the positions of the C atoms with an open square.

5. (8 points) Construct the primitive reciprocal lattice vectors for this crystal and on the graph below sketch the vectors and plot the positions of the reciprocal lattice points by marking them with a ×.

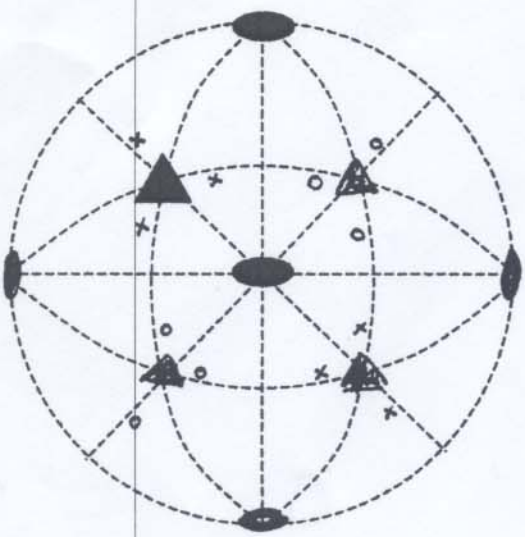
6. (8 points) On the same plot, indicate the points at which you expect to see diffaction from peaks with contributions from both the Si and C atoms. Indicate these spots with an open circle.

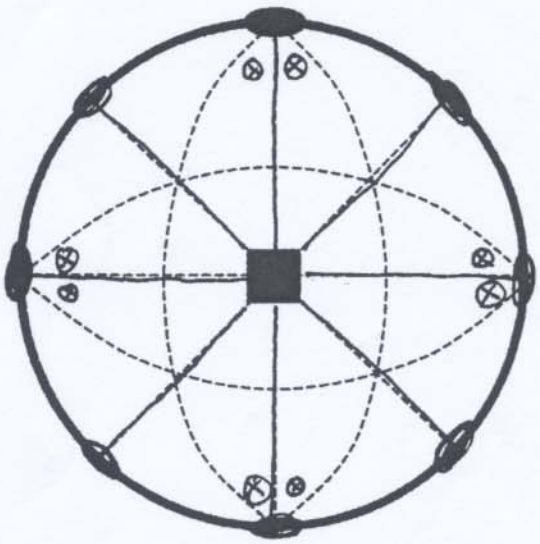


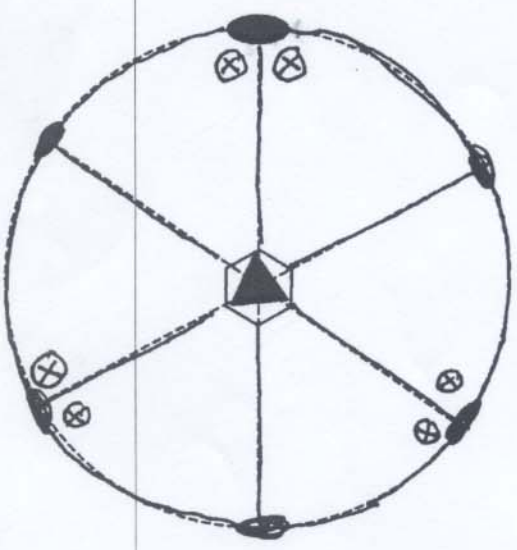
- From the table we see no condition for Wyckoff letter 'a'. Therefore we expect that site 'a' will have a diffraction spot at each lattice point.

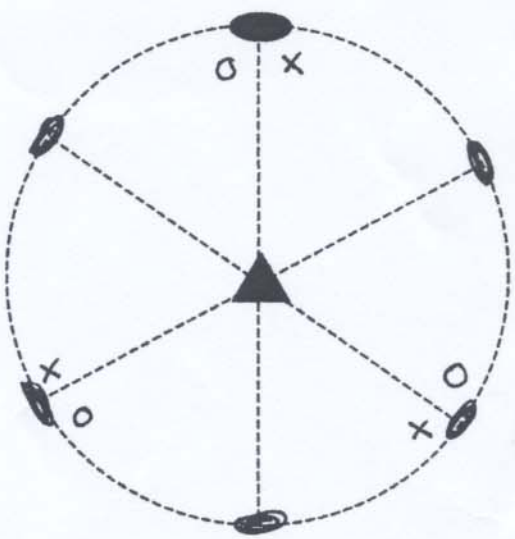
- Wyckoff site c → $h+k=2n$. At positions were h+k sum to an even # will yield a diffraction pattern.

2. (8 points each) Complete the following stereograms. Indicate all symmetry elements on the stereogram (no need to list them explicitly), and which points (directions) are equivalent by symmetry. Pick a point that does *not* lie on a symmetry element.





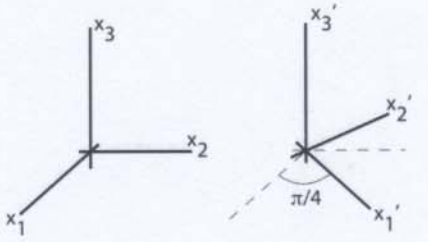




outcome 5

3. Two coordinate systems are related as shown below. In the primed frame, the distortion tensor has the components:

$$\mathbf{e}' = \begin{bmatrix} 0 & 2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$



a. (5 points) Give the components of the *strain* tensor in the primed frame. Recall that the strain tensor is the symmetric part of the distortion tensor.

$$\varepsilon'_{ij} = \frac{1}{2}(e_{ij} + e_{ji}) = \begin{bmatrix} \frac{1}{2}(e_{11}+e_{11}) & \frac{1}{2}(e_{12}+e_{21}) & \frac{1}{2}(e_{13}+e_{31}) \\ \frac{1}{2}(e_{21}+e_{12}) & \frac{1}{2}(e_{22}+e_{22}) & \frac{1}{2}(e_{23}+e_{32}) \\ \frac{1}{2}(e_{31}+e_{13}) & \frac{1}{2}(e_{32}+e_{23}) & \frac{1}{2}(e_{33}+e_{33}) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

b. (5 points) Give the matrix that transforms the coordinates from the unprimed to the primed frame.

$$a = \begin{pmatrix} \cos x_1' x_1 & \cos x_1' x_2 & \cos x_1' x_3 \\ \cos x_2' x_1 & \cos x_2' x_2 & \cos x_2' x_3 \\ \cos x_3' x_1 & \cos x_3' x_2 & \cos x_3' x_3 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\frac{\pi}{4} & \cos\frac{\pi}{2} & 0 \\ \cos\frac{\pi}{2} & \cos\frac{\pi}{4} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

c. (5 points) Give the components ε_{11} and ε_{22} of the strain tensor in the unprimed frame. (The primed frame is rotated about the x_3 axis by and angle $\pi/4$ as shown.)

$$\varepsilon_{kl} = a_{ik}\, a_{jl}\, \varepsilon'_{ij}$$

$$\varepsilon_{11} = a_{i1}\, a_{j1}\, \varepsilon'_{ij}$$

$$= a_{11} a_{j1} \varepsilon_{1j} + a_{21} a_{j1} \varepsilon_{2j} + a_{31} a_{j1} \varepsilon_{3j}$$

$$= a_{11}a_{11}\varepsilon_{11} + a_{11}a_{21}\varepsilon_{12} + a_{11}a_{31}\varepsilon_{13} + a_{21}a_{11}\varepsilon_{21} + a_{21}a_{21}\varepsilon_{22} + a_{21}a_{31}\varepsilon_{23}$$

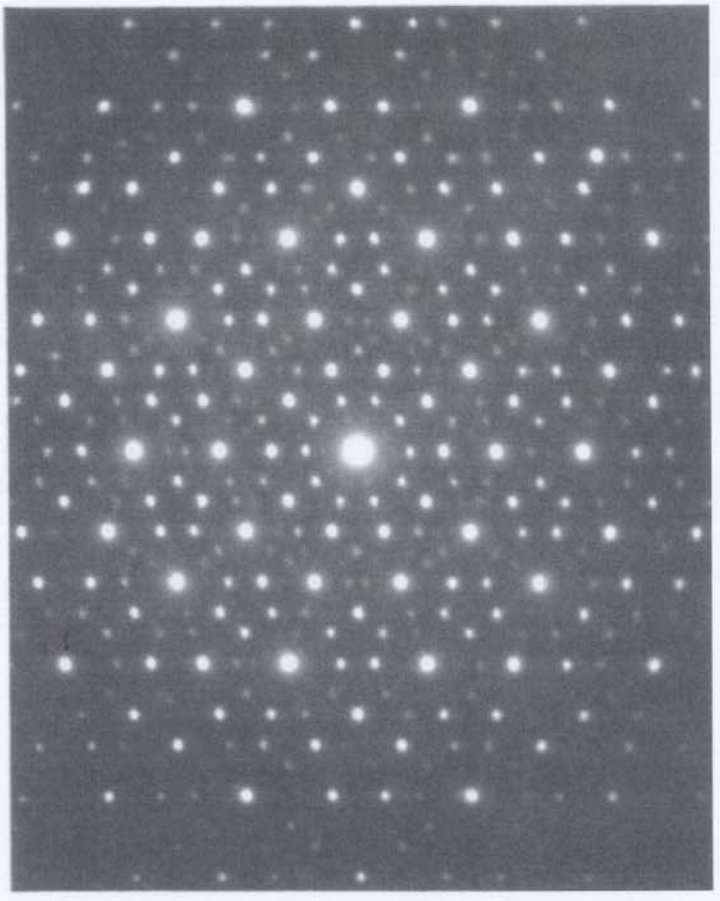
$$+ a_{31}a_{11}\varepsilon_{31} + a_{31}a_{21}\varepsilon_{32} + a_{31}a_{31}\varepsilon_{31}$$

The same approach for ε_{22}. Many terms will fall out because of $\emptyset$.

outcome 6

4. (5 points) The image below is a diffraction pattern obtained from a solid. (The image is obtained with transmission electron microscopy – however the diffraction principles are basically the same as for x-ray diffraction.) The discovery of materials with diffraction patterns like this in 1984 caused quite a stir in the materials community.

What is unusual about it? (This pattern is slightly different from what we have considered, as it stems from a 3-D experiment. Nevertheless, you should be able to draw some interesting conclusions.)



The symmetry around the central point shows a 10 fold axis of rotation.