MSE 102, Fall 2009

Midterm #1

Write your name here: Solutions

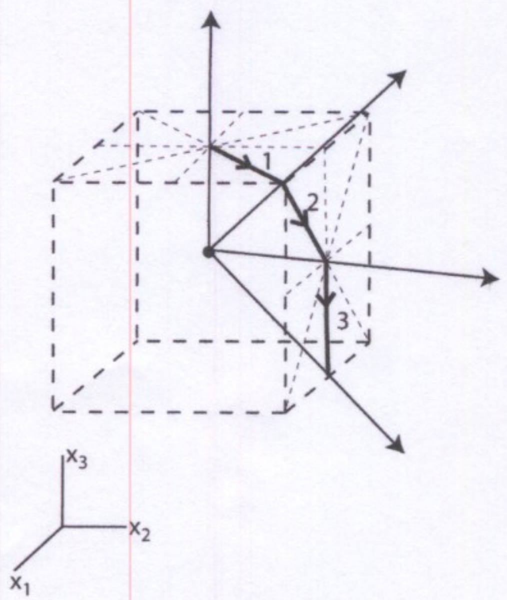
Instructions:

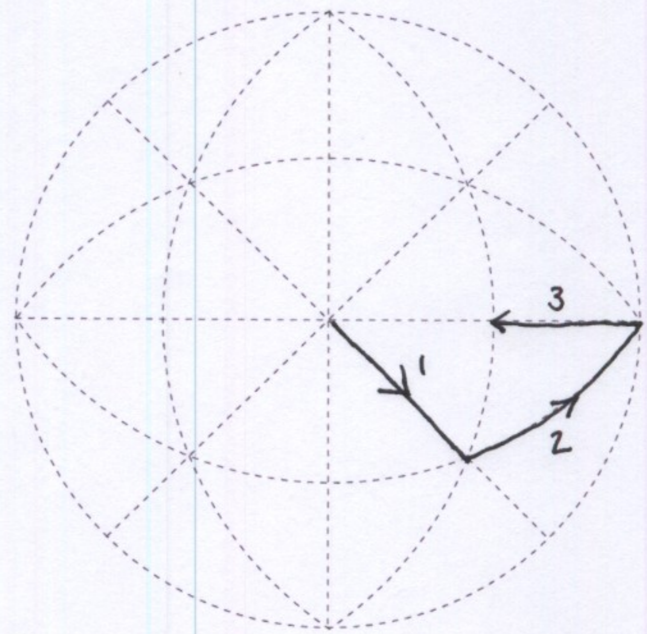
- Answer all questions to the best of your abilities. Be sure to write legibly and state your answers clearly.
- The point values for each question are indicated.
- You are not allowed to use notes, friends, phones, consultants, employees, etc.
- There are a total of 100 points. You get 3 point for just showing up, the remaining 97 you have to earn.
- Feel free to ask questions, but only for clarification purposes.

This exam constitutes can contribute up to 20% of the points accrued toward your final grade, as stated in the syllabus. Good luck. I sincerely hope you all do really well.

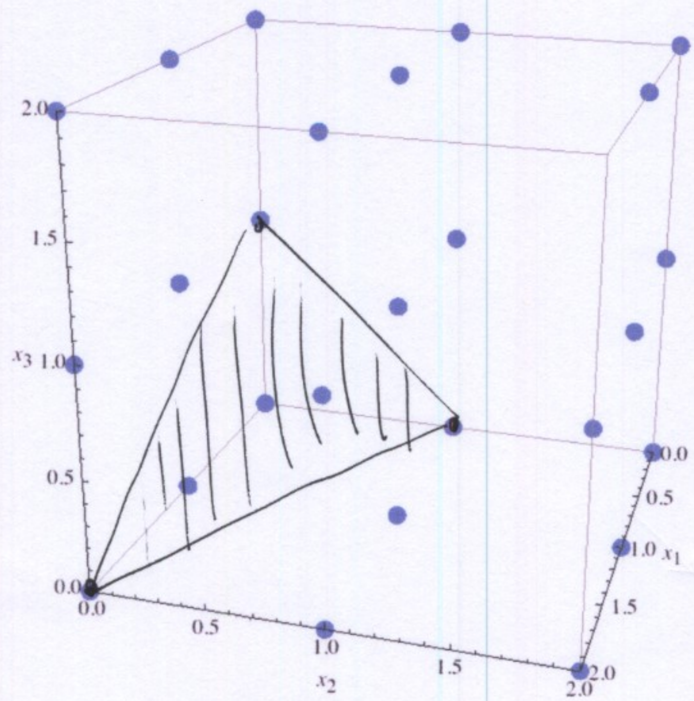
-Prof. Chrzan

(1) [5 points] Assume that a ray emanates from the center of the cube as shown. Suppose that it changes direction, and as it moves it traces the path shown as a solid line on the surface of the cube. Map the path onto the stereogram on the right using your understanding of the stereographic projection. Label each segment of the path with the number shown on the cube.





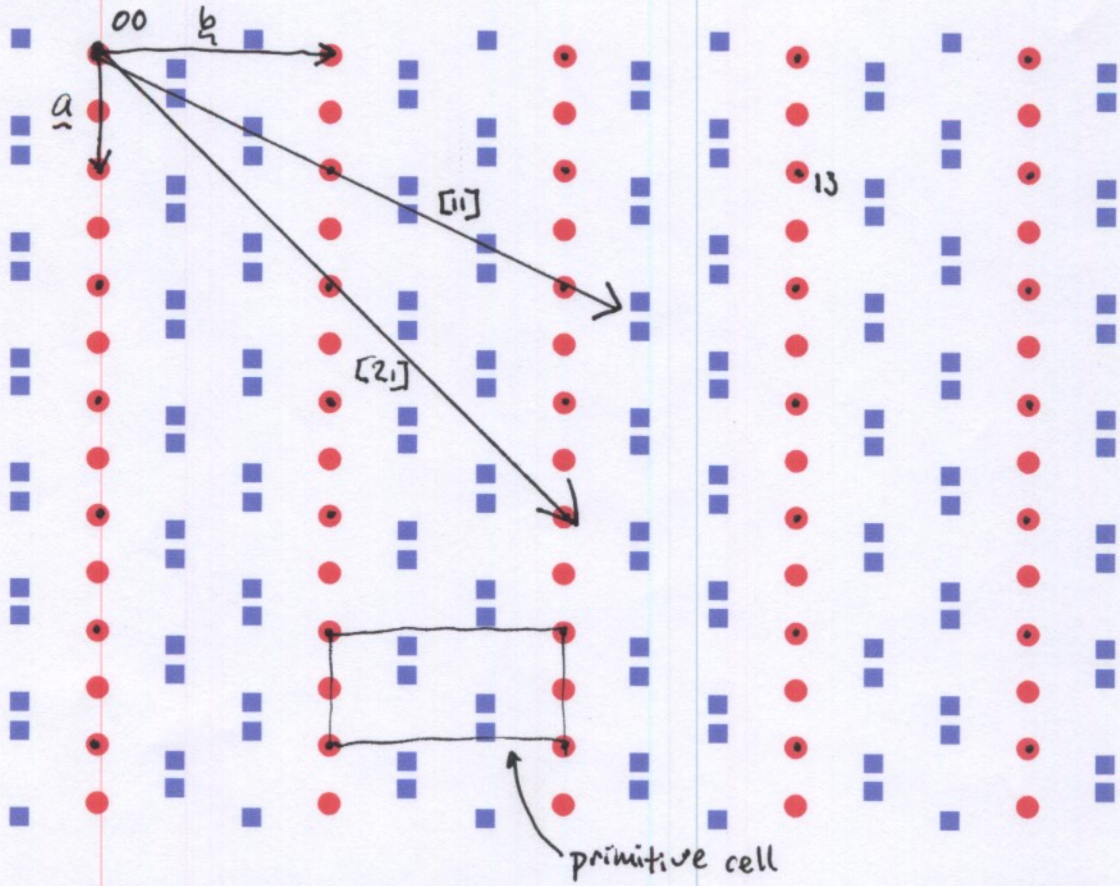
(2) [5 points] A portion of a simple cubic lattice is plotted below. Use this plot to sketch the plane that intersects the x_1 axis at 2, the x_2 axis at 1 and the x_3 axis at 1. Give the Miller indices of the plane that you sketched.



The Miller indices are defined by the reciprocals of the intercepts:

$$h:k:l = \frac{1}{2} : \frac{1}{1} : \frac{1}{1}$$

$$\therefore \quad (hkl) = (1\,2\,2)$$



(32) (3) A portion of a two dimensional crystal is shown above. The circles represent one type of atom, the squares another.

(a) [4 points] On the figure above, identify a set of primitive lattice vectors. Draw a dot at each lattice point.
(b) [4 points] Indicate the point 00 (place this in the upper left hand corner for convenience) and identify the point 13.
(c) [4 points] Draw the direction [21].
(d) [4 points] On the figure above, identify a primitive unit cell.
(e) [4 points] How many atoms (total, irrespective of type) are associated with each primitive unit cell?

6 atoms – 4 square + 2 circle

(f) [4 points] Identify the plane group name and/or number describing the symmetry of this crystal.

p2mg – No. 7

(g) [4 points] Give the Wyckoff letter corresponding to the atoms represented by circles.

a

(h) [4 points] Give the Wyckoff letter corresponding to the atoms represented by squares.

d

(4) A 2-D crystal has an atomic scale structure described by the symmetry group *pg* (plane group No. 4). The lattice parameters are a=π and b=2π. There are atoms at Wyckoff position(s) *a* with x=y=1/4.

(a) [5 points] Find the primitive reciprocal lattice vectors and give and define $\mathbf{G}_{hk}$ in terms of integers *h* and *k* for all the reciprocal lattice vectors of this lattice.

$\underset{\sim}{a} = (0, -\pi) \qquad \underset{\sim}{b} = (2\pi, 0)$

$\underset{\sim}{a}^* \cdot \underset{\sim}{a} = 2\pi \qquad \underset{\sim}{a}^* \cdot \underset{\sim}{b} = 0 \qquad \Rightarrow \qquad \underset{\sim}{a}^* = (0, -2), \ \underset{\sim}{b}^* = (1, 0)$

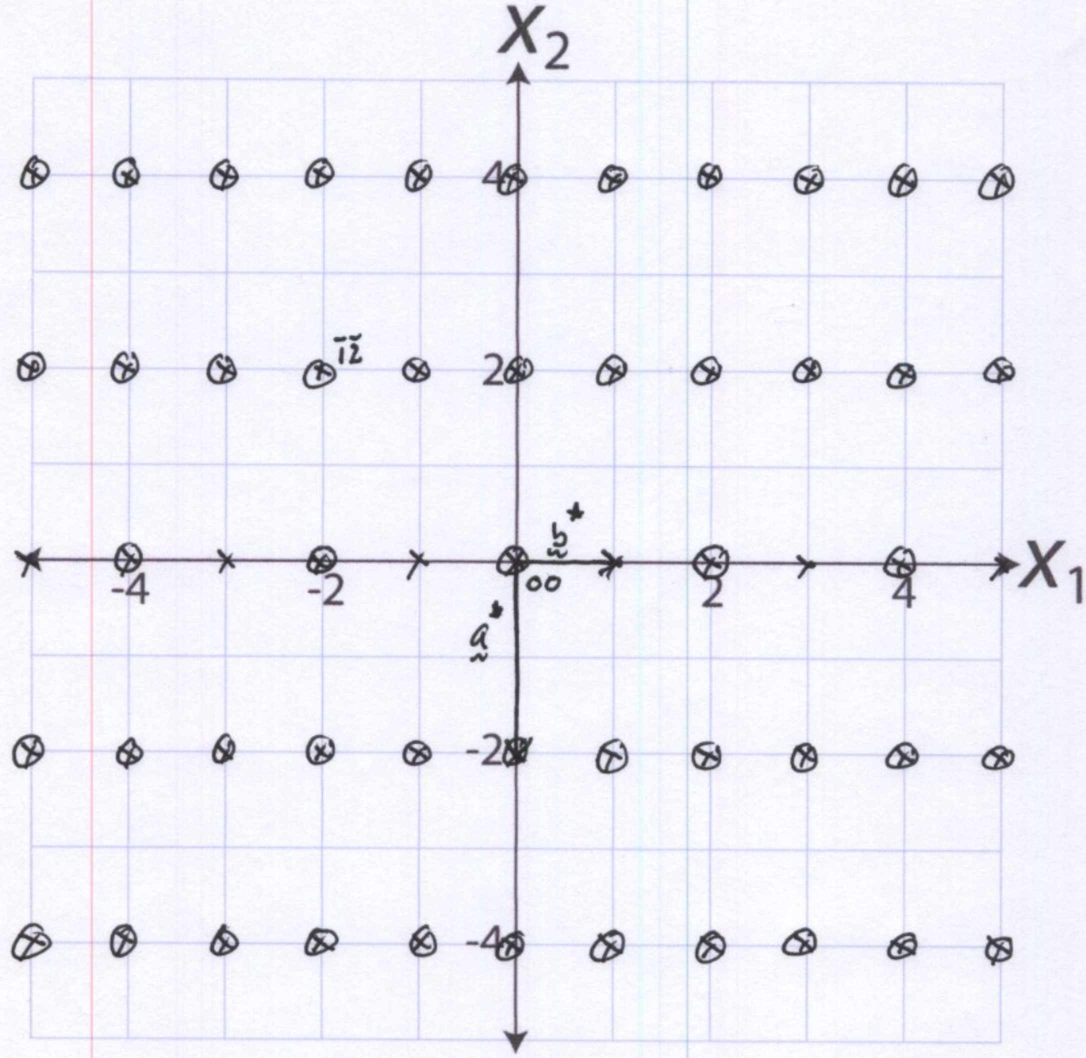
$\underset{\sim}{b}^* \cdot \underset{\sim}{a} = 0 \qquad \underset{\sim}{b}^* \cdot \underset{\sim}{b} = 2\pi$

$\underset{\sim}{G}_{hk} = h\underset{\sim}{a}^* + k\underset{\sim}{b}^*.$

(b) [5 points] On the attached graph paper, sketch $\underset{\sim}{a}^*$ and $\underset{\sim}{b}^*$ and plot the reciprocal lattice points using an ×. Label the points 00 and $\bar{1}\bar{2}$.

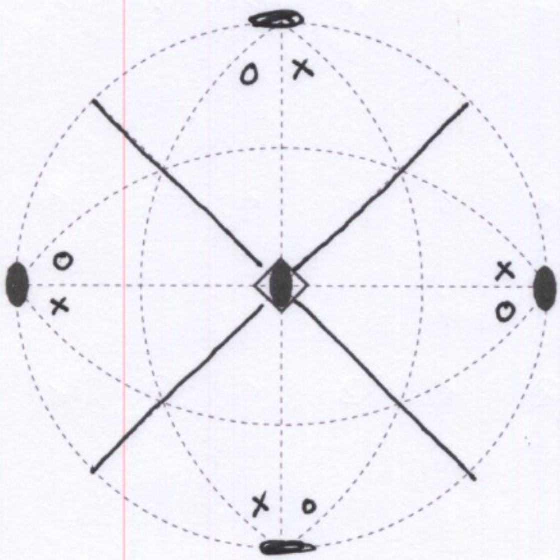
(c) [5 points] On the same plot, indicate the reciprocal lattice spots that will correspond to the bright reflections during an x-ray diffraction experiment using an ○.

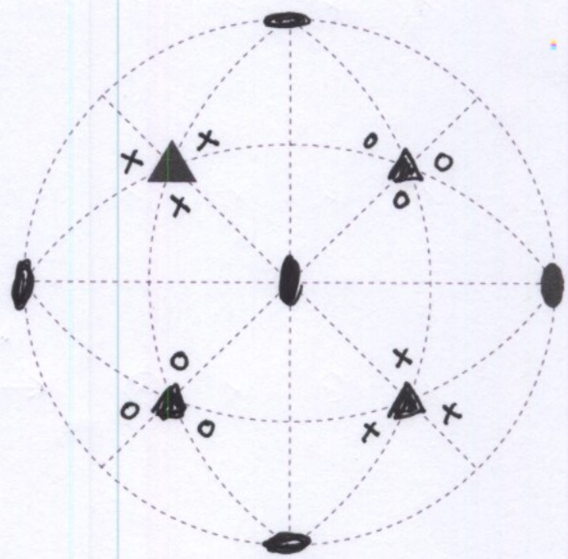
Based on the plane group tables, the conditions are stated 0k: k=2n. Therefore along the h=0 axis, only even spots yield Bragg reflections.

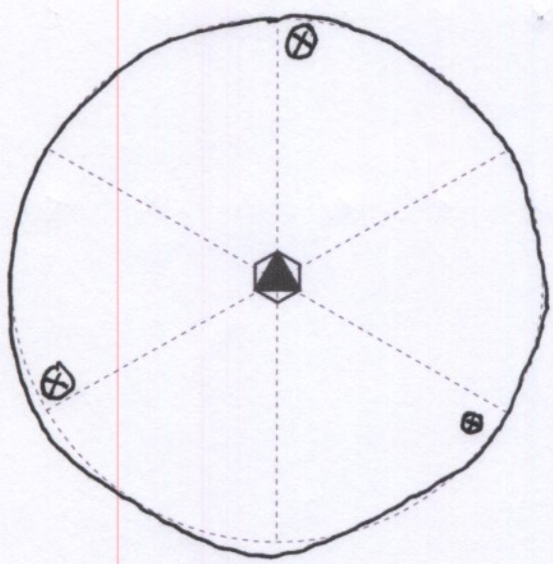


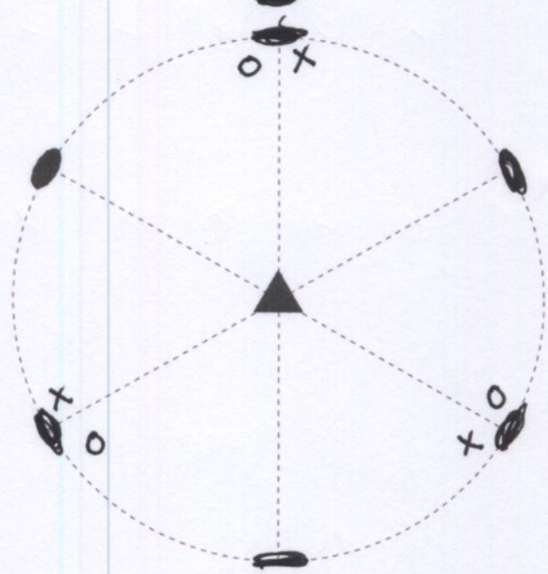
X_2
X_1
4
2
-2
-4
-4
-2
2
4
$\tilde{12}$
b^*
a^*
00

(5) [5 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.









(6) Two coordinate systems, describing a primed and unprimed frame, are defined by the unit vectors:

$$\begin{aligned}
\mathbf{e}_1 &= 1\mathbf{e}_x + 0\mathbf{e}_y + 0\mathbf{e}_z \quad & \mathbf{e}_1' &= \frac{1}{\sqrt{6}}\mathbf{e}_x + \frac{1}{\sqrt{6}}\mathbf{e}_y - \sqrt{\frac{2}{3}}\mathbf{e}_z \\
\mathbf{e}_2 &= 0\mathbf{e}_x + 1\mathbf{e}_y + 0\mathbf{e}_z \quad & \mathbf{e}_2' &= -\frac{1}{\sqrt{2}}\mathbf{e}_x + \frac{1}{\sqrt{2}}\mathbf{e}_y + 0\mathbf{e}_z \ . \\
\mathbf{e}_3 &= 0\mathbf{e}_x + 0\mathbf{e}_y + 1\mathbf{e}_z \quad & \mathbf{e}_3' &= \frac{1}{\sqrt{3}}\mathbf{e}_x + \frac{1}{\sqrt{3}}\mathbf{e}_y + \frac{1}{\sqrt{3}}\mathbf{e}_z
\end{aligned}$$

Here, $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$ are the unit vectors of the Cartesian coordinate system.

(a) [5 points] Give the matrix **a** that transforms from the *unprimed* frame to the *primed* frame: We note that $a_{ij} = \underset{\sim}{e}_i' \cdot \underset{\sim}{e}_j$. Therefore

$$\underline{\underline{a}} = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{\sqrt{2}}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix}$$

(b) [5 points] Give (using Einstein notation and the definition of the matrix **a** as the matrix that transforms from the unprimed to the primed frame) the general equation that transforms a second rank tensor in the primed frame into the unprimed frame.

$$T_{ij} = a_{ki}\, a_{\ell j}\, T'_{k\ell}$$

(b) [5 points] In the primed frame, a certain second rank tensor has the components:

$$\sigma' = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Transform this tensor to the unprimed frame defined by the unit vectors given above.

This problem just requires that one do the algebra. It is straightforward, and a pattern emerges quickly.

$$\sigma_{11} = a_{k1} a_{l1} \sigma'_{kl} = a_{31}^2 \sigma'_{33} = \frac{1}{3}$$

$$\sigma_{12} = a_{k1} a_{l2} \sigma'_{kl} = a_{31} a_{32} \sigma'_{33} = 1/3$$

$$\sigma_{13} = a_{k1} a_{k3} \sigma'_{kl} = a_{31} a_{33} \sigma'_{33} = 1/3$$

$$\sigma_{21} = a_{k2} a_{l1} \sigma'_{kl} = a_{32} a_{31} \sigma'_{33} = 1/3$$

$$\sigma_{22} = a_{k2} a_{l2} \sigma'_{kl} = a_{32}^2 \sigma'_{33} = 1/3$$

$$\sigma_{23} = a_{k2} a_{l3} \sigma'_{kl} = a_{32} a_{33} \sigma'_{23} = 1/3$$

$$\sigma_{31} = a_{k3} a_{l1} \sigma'_{kl} = a_{33} a_{31} \sigma'_{33} = 1/3$$

$$\sigma_{32} = a_{k3} a_{l2} \sigma'_{kl} = a_{33} a_{32} \sigma'_{33} = 1/3$$

$$\sigma_{33} = a_{k3} a_{l3} \sigma'_{kl} = a_{33}^2 \sigma_{33} = 1/3$$

$$\therefore \quad \underset{\approx}{\sigma} = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}.$$

Alternatively, one can write:

$$\sigma_{ij} = a_{ki} a_{lj} \sigma'_{kl}$$

for this case only $\sigma'_{33} \neq 0$. $\therefore$ $\sigma_{ij} = a_{3i} a_{3j} \sigma'_{33}$

$$\sigma_{ij} = \frac{1}{3}.$$