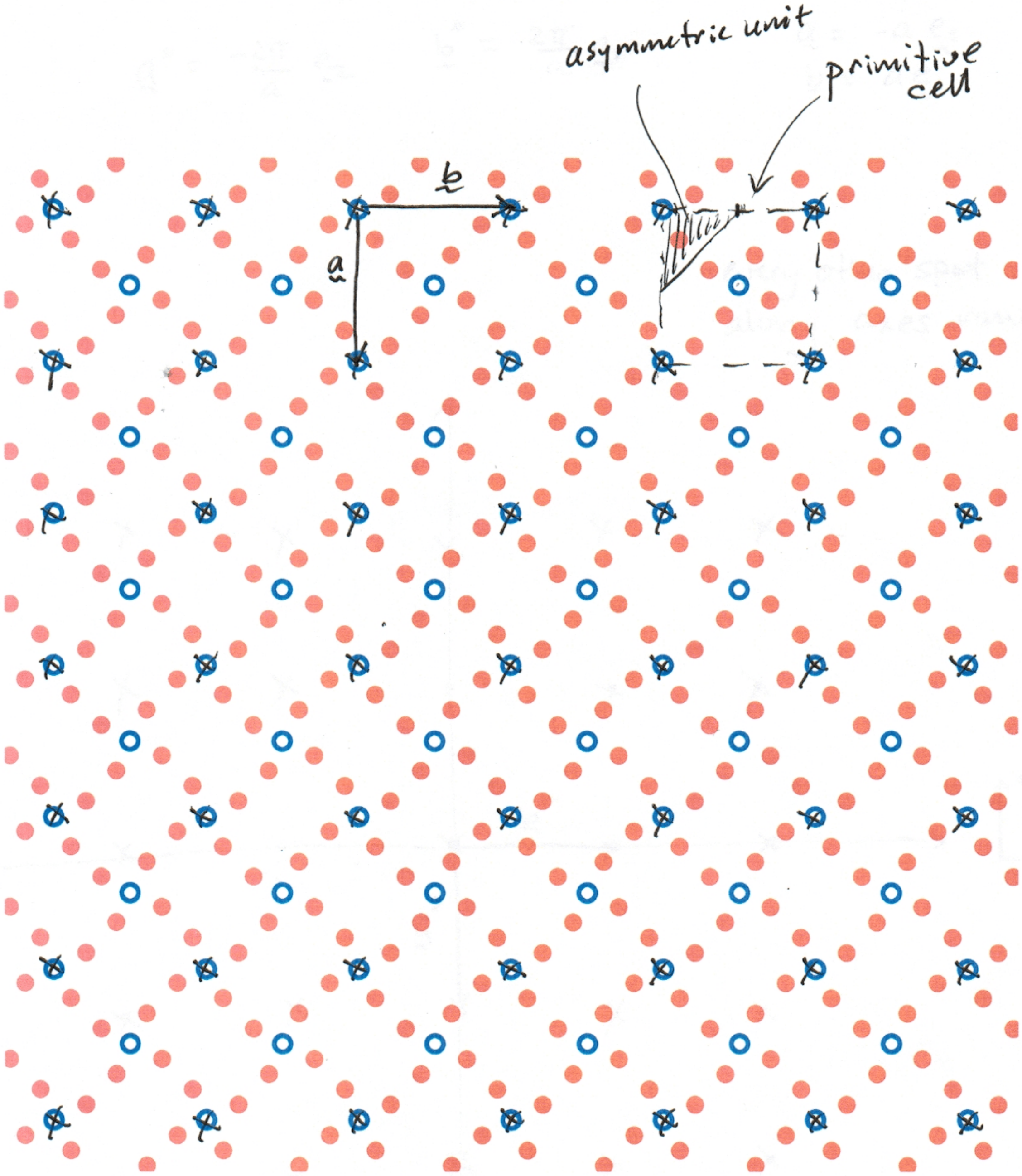
Problem 1. [Total of 55 points] The structure below is a 2D crystal. It includes two types of atoms, indicated by filled and open circles. (The atoms have spherical symmetry.) On the figure:

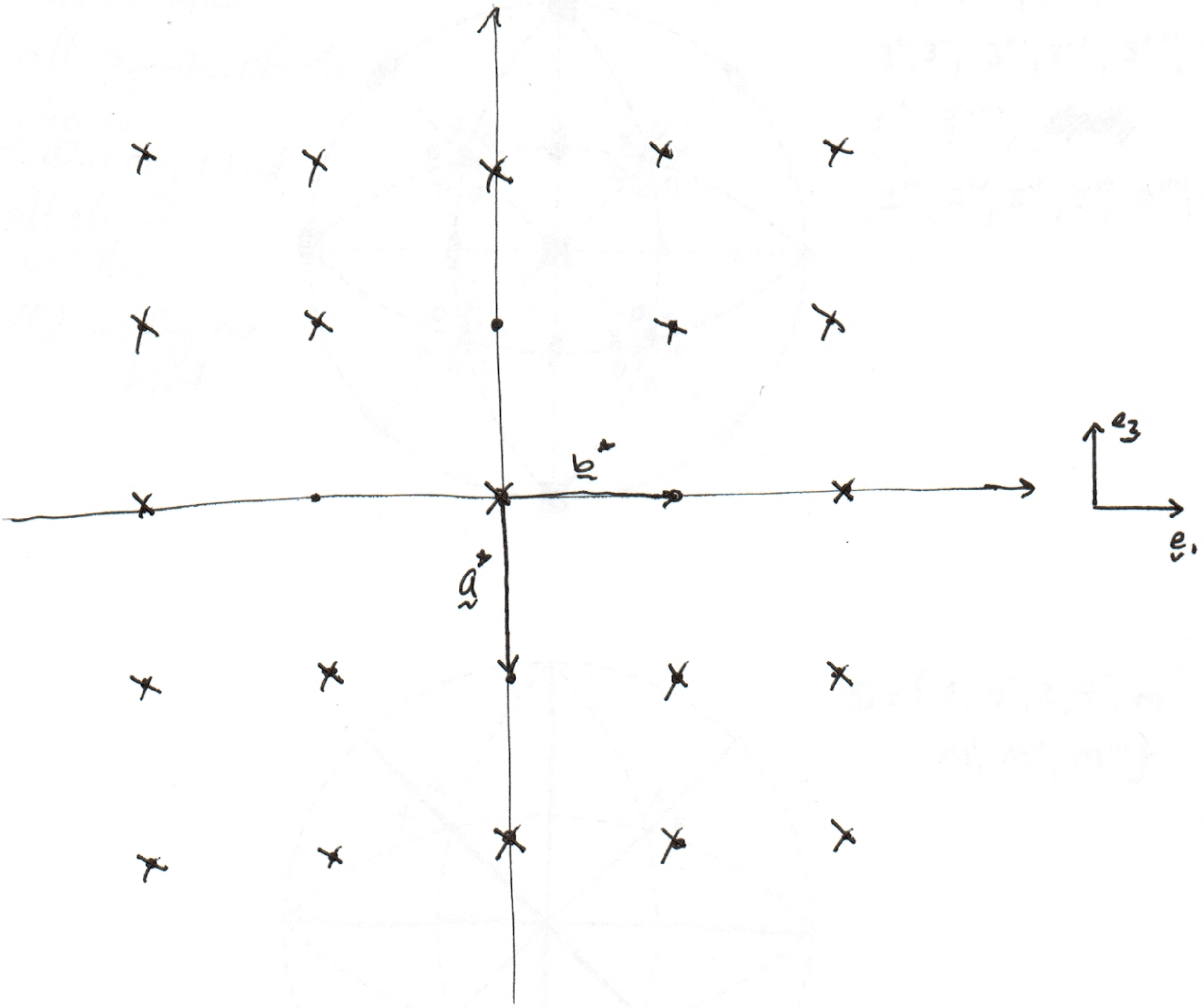
a. [5 points] Place an × at the positions of the lattice points.
b. [5 points] Identify a set of primitive lattice vectors for the crystal.
c. [5 points] Identify a primitive unit cell.
d. [5 points] How many atoms are in the primitive unit cell? 10
e. [5 points] Which plane group describes the symmetry of this crystal? p4gm
f. [5 points] Identify the asymmetric unit for this crystal.
g. [5 points] Give the Wyckoff letter for the positions of the atoms indicated by filled circles. d
h. [5 points] Give the Wyckoff letter for the positions of the atoms indicated by open circles. a
i. [5 points] Based on the International Tables, at which reciprocal lattice points *hk* will the atoms indicated by open circles give contributions to the x-ray diffraction pattern? h0: h=2n, 0k: k=2n and hk: h+k=2n
j. [5 points] Based on the International Tables, at which reciprocal lattice points *hk* will the atoms indicated by filled circles give a contribution to the x-ray diffraction pattern? h0: h=2n 0k: k=2n
k. [5 points] On the blank page following the plot of the atoms, define the unit vectors $\mathbf{e}_1$ and $\mathbf{e}_2$. Draw the reciprocal lattice vectors $\mathbf{a}^*$ and $\mathbf{b}^*$, and place a dot at each reciprocal lattice vector. Now place an × at each point for which you expect to see a spot in the x-ray diffraction pattern.

a) 5 either set
b) 5 any primitive lattice vectors
c) 5 any primitive lattice cell
d) 5 10
e) 5 p4gm
→ 2 correct symmetry elements
→ +1 P4 series
f) 5 draw correctly (as long same area)
→ 3 list conditions but draw different from condition
→ 0 list condition
g) 5 d → 1 for most general point
h) 5 a → 2 if also has 4.. symmetry
i) 5 full pattern
i) → 2 only hk: h+k=2
j) 5 full condition
k) 1 $|\underline{a}^*| = |\underline{b}^*|$
+1 $\underline{a}^* \perp \underline{b}^*$
+1 explain why $|a^*| = |$
+1 alternate axes
+1 everything else light up


asymmetric unit
primitive cell
a
b

$$\underset{\sim}{a}^* = \frac{-2\pi}{a}\,\underset{\sim}{e}_2 \qquad \underset{\sim}{b}^* = \frac{2\pi}{a}\,\underset{\sim}{e}_1 \qquad \begin{aligned}\underset{\sim}{a} &= -a\,\underset{\sim}{e}_2 \\ \underset{\sim}{b} &= a\,\underset{\sim}{e}_1\end{aligned}$$

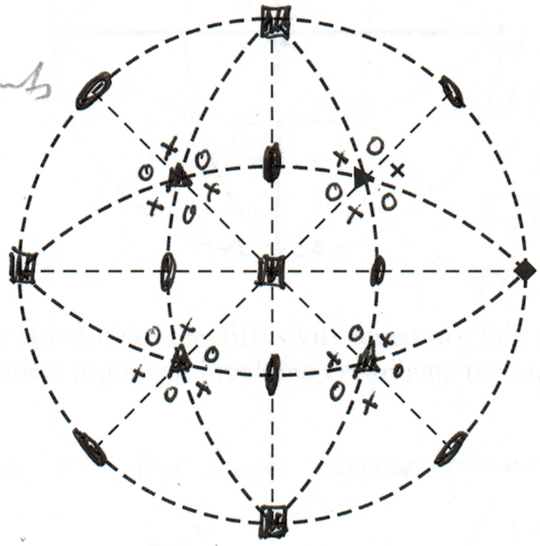
every other spot
along axes vanishes



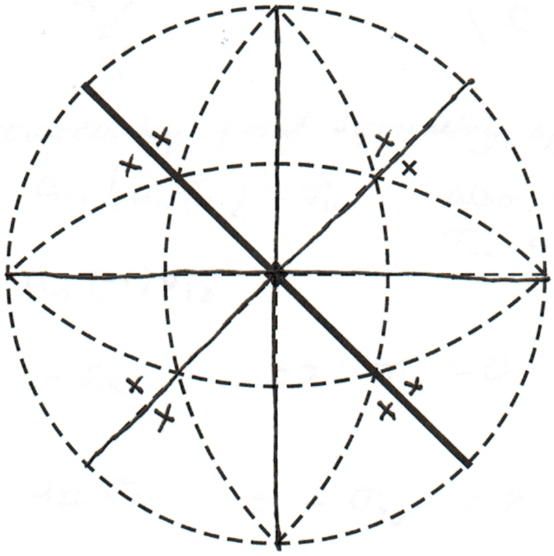
2. [5 points each] Complete the stereographic projections for the point groups shown below using the given direction as one of the directions that is equivalent by symmetry. Enumerate all the symmetry elements of the point group.

① all direction
+ ② all symmetry elements drawn
→ ① missing 1 kind
+ ②. all elements written
→ ① missing one kind

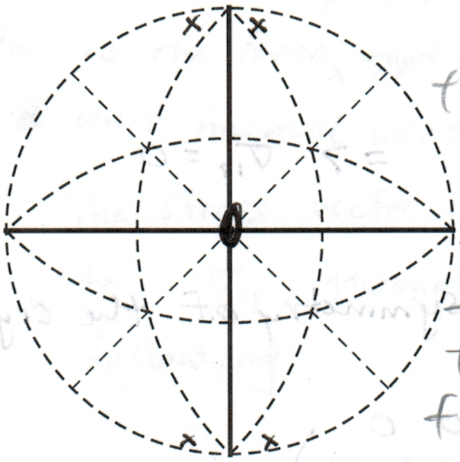
$G = \{ 1, 4^+, 2, 4^-,$
$4^{+'}, 2', 4^{-'}, 4^{+''}, 2'', 4^{-''}$
$3^+, 3^-, 3^{+'}, 3^{-'}, 3^{+''}, 3^{-''},$
$3^{+'''}, 3^{-'''},$
$2''', 2^{iv}, 2^{v}, 2^{vi}, 2^{vii}, 2^{viii} \}$



$G = \{ 1, 4^+, 2, 4^-, m,$
$m', m'', m''' \}$



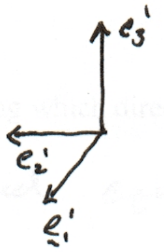
Problem 3. A crystal is known to have the point symmetry shown below.



(2) Fick's first law to prove second rank
+ (2) Transformation rule/equation
→ (1) Transformation rule for other rank
+ 2×(2) For any 2 correct a_{ij}
+ (1) Onsager
+ 2×(2) for correct ways of each a_{ij}
+ (1) correct answer
+ (1) mention that all symmetry elements considered or explain clearly why only 2 of that required

[15 points] What is the structure of the diffusivity tensor for this material? Justify your answer with a mathematical argument involving coordinate transformations.

Consider the action of the first mirror plane.



$$\underline{\underline{a}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Because frames are related by point symmetry operation, we have:

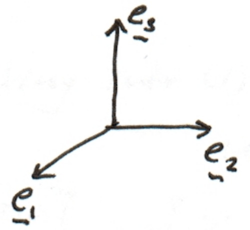
$\sigma_{11} = \sigma_{11}' = a_{1i}a_{1j}\sigma_{ij} = a_{1i}(a_{11}\sigma_{i1}) = \sigma_{11}$ also no constraints on σ_{22} and σ_{33}.

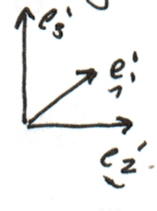
$\sigma_{12} = \sigma_{12}' = a_{1i}a_{2j}\sigma_{ij} = a_{1i}(-1)\sigma_{i2}$

$= -\sigma_{12} \Rightarrow \sigma_{12} = 0$

$\sigma_{23} = \sigma_{23}' = a_{2i}a_{3j}\sigma_{ij} = a_{2i}\sigma_{i3} = -\sigma_{23} \Rightarrow \sigma_{23} = 0$

The second mirror plane is aligned along y-axis (e_2).





$$\underline{\underline{a}} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\sigma_{13} = \sigma'_{13} = a_{1i}\, a_{3j}\, \sigma_{ij}$$

$$= a_{1i}\, \sigma_{i3}$$

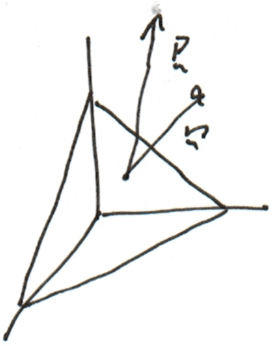
$$= -\sigma_{13} \qquad \Rightarrow \quad \sigma_{13} = 0$$

So based on the symmetry of the crystal

$$\underset{\sim}{\sigma} = \begin{pmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{pmatrix}.$$

Problem 4. [5 points] What is the stress vector and how is it related to the stress tensor?

The stress vector is the force per unit area applied across a plane with unit normal vector $\underset{\sim}{n}$.



The stress vector is related to σ_{ij} through the following

$$P_i = \sigma_{ij} n_j .$$

(1) Force/area applied OR (3) Clear diagram
+ (1) plane/face
+ (1) unit normal $\underline{n}$
+ (2) equation
→ OR (1) Second rank tensor.
+ (1) multiplied with n to give p

Problem 5. [5 points] Along which direction do the planes (111) and (123) intersect?

Using the zonal equation we have

(2) Zone law stated or equation written
OR Any other Correct methods + (2) Correct application + (1) $(1\bar{2}1)$

(1) $u + v + w = 0$

(2) $u + 2v + 3w = 0$

Solving (1) for u and substituting into (2) we find:

$$-v - w + 2v + 3w = 0$$

$$+v + 2w = 0$$

$$v = -2w$$

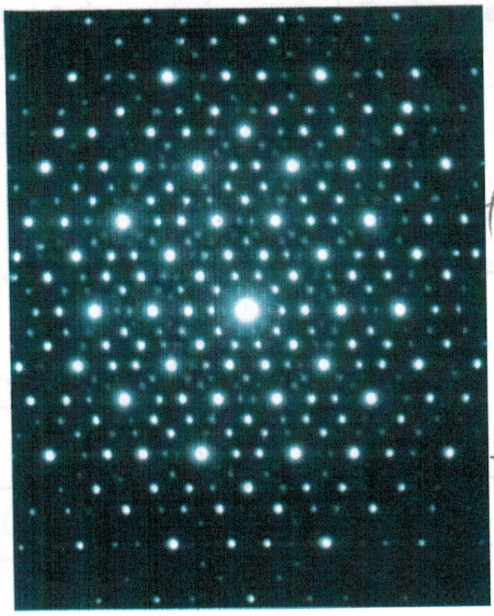
substituting into (1)

$$u - 2w + w = 0 \quad \Rightarrow u = w$$

$\therefore$ $[uvw] = [w\ {-2w}\ w] \Rightarrow [1\ \bar{2}\ 1]$

direction of intersection

Problem 6. [5 points] The x-ray diffraction pattern from a quasicrystal is shown in the image below. Based on our discussions in class, what is unusual about this diffraction pattern?



(2) 10/5 fold

+(2) Not allowed in lattices discussed

OR cannot be translated

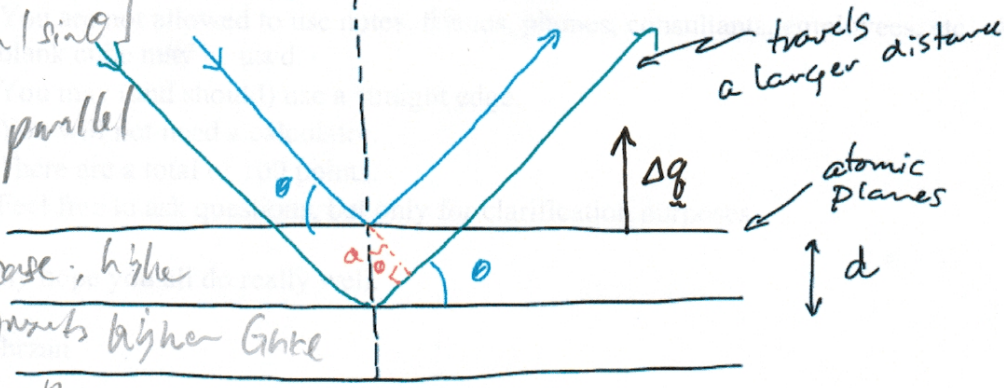
+(1) If not present in real space, also not present in reciprocal space

This diffraction pattern appears to have a 10-fold (2) axis of symmetry. There is no lattice that allows (2) for a 10-fold axis of symmetry, so this pattern cannot correspond to a reciprocal lattice

(1)

Problem 7. [5 points] In class, we derived the condition that constructive interference yielding a bright spot in an x-ray diffraction pattern will be observed whenever $\Delta\mathbf{q} = \mathbf{G}_{hkl}$ with $\Delta\mathbf{q}$ the scattering vector and $\mathbf{G}_{hkl}$ a reciprocal lattice vector. We also derived the Bragg conditions for scattering $n\lambda = 2d\sin\theta$, with λ, the wavelength of the x-rays, d the spacing between planes, and θ the scattering angle defined in the figure. Explain how these two conditions are the same.

① $|G_{hkl}| = \frac{2\pi}{d_{hkl}}$ } for amplitude
+① $|\Delta q| = 2|q_{in}|\sin\theta$
+① G_{hkl} & Δq parallel for direction
+① For $n \neq 1$ case, higher n just represents higher G_{hkl}
+① Correct math.



In the geometry of the Bragg diffraction analysis, $\underset{\sim}{\Delta q}$ points normal to the lattice planes. Suppose that the lattice planes in question are the (hkl) planes. Then we know that $\underset{\sim}{G}_{hkl}$ points normal to these planes as well, so that $\underset{\sim}{G}_{hkl}$ and $\underset{\sim}{\Delta q}$ are parallel. Based on the Bragg scattering geometry ①

$$|\Delta \underset{\sim}{q}| = 2|\underset{\sim}{q}_{in}|\sin\theta = 2\left(\frac{2\pi}{\lambda}\right)\sin\theta. \quad ①$$

We also have that $|\underset{\sim}{G}_{hkl}| = \frac{2\pi}{d_{hkl}}$. ① Noting that since

~~Δq~~ $\Delta \underset{\sim}{q} = \underset{\sim}{G}_{hkl} \Rightarrow |\Delta \underset{\sim}{q}| = |\underset{\sim}{G}_{hkl}|$, we have

① $\frac{2\pi}{d_{hkl}} = 2\left(\frac{2\pi}{\lambda}\right)\sin\theta$, rearranging gives the

Bragg criteria for $n=1$: $\lambda = 2d_{hkl}\sin\theta$, so the two conditions are the same for $n = 1$. Higher values of n in Bragg's law correspond to different $\underset{\sim}{G}_{hkl}$'s. Noting that $\underset{\sim}{G}_{nh\,nk\,nl} = n\,\underset{\sim}{G}_{hkl}$ makes this apparent.

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