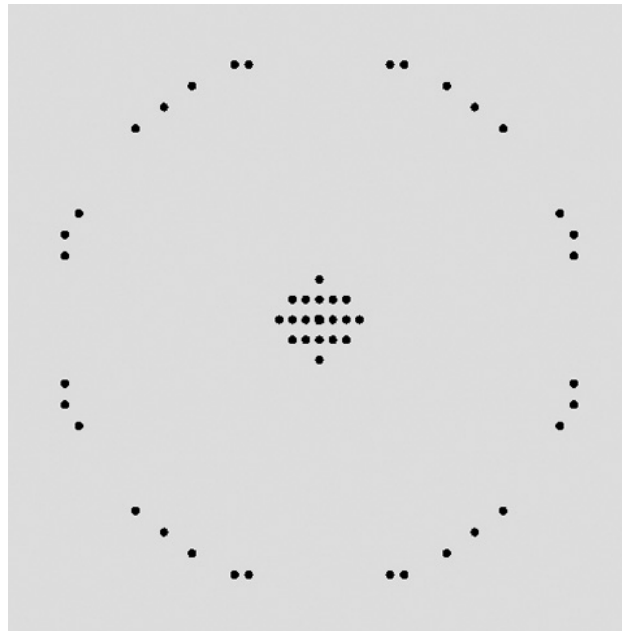


Problem Set #5:

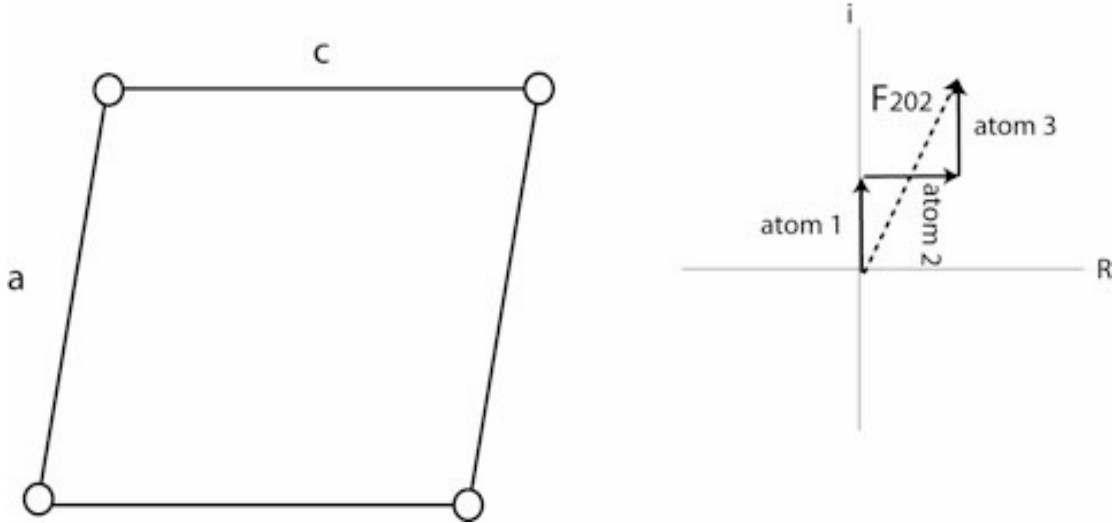
1. In a few sentences, explain why the x-ray diffraction pattern obtained from a protein crystal appears as discrete reflections instead of a continuum. What information is encoded by the positions of the reflections? What is encoded by the relative intensities of reflections?

2. Bragg's law states that for two x-rays to scatter in phase, the condition $\lambda = 2d \sin \theta$ must be satisfied. For the diffraction image below, the detector was positioned 200 mm from the crystal and $\lambda = 1.5 \text{ \AA}$. What unit cell dimensions can be derived from the spacings of reflections within the central zone on this diffraction image ($a^* = 7/4 \text{ mm}$ [horizontal direction]; $b^* = 10/4 \text{ mm}$ [vertical direction])?

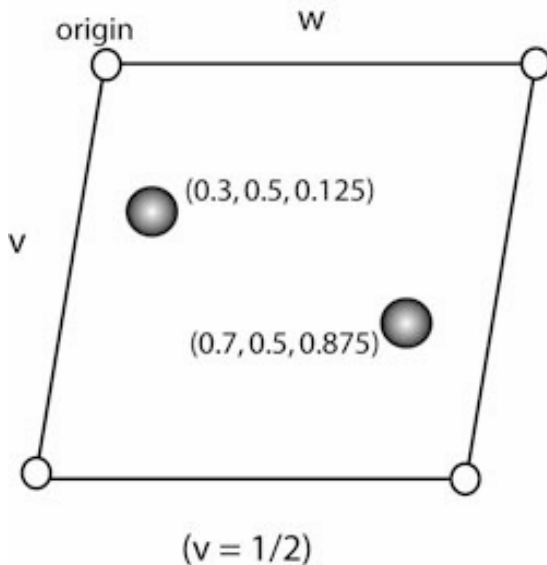


3. What is the unit cell dimension ($c = ?$) parallel to the x-ray beam? (Hint: calculate the 2θ angle for the lune of reflections [33 mm radius] surrounding the central zone then consider the geometry of Ewald's sphere)

4. On the following drawing of a unit cell, draw the Bragg reflection planes corresponding to Miller indices $(hkl = 202)$. Draw 3 atoms with positions in the unit cell that are consistent with the vector diagram shown for the F_{202} reflection.



5. The space group $P2_1$ has one Harker section located at $v = 1/2$. Using the symmetry operators below, write the Harker vector equation(s) and calculate the atomic coordinates ($x = ?$; $z = ?$) for the heavy atom site corresponding to the peak shown below.



Symmetry for $P2_1$:
 (X, Y, Z)
 $(-X, Y+1/2, -Z)$

6. Describe in physical terms what is meant by “crystal mosaic spread” (mosaicity) and explain how it affects the diffraction pattern of a crystal, leading to inaccurate x-ray intensity measurements.

7. The protein phase estimate (ϕ_p) for each reflection calculated from a single heavy atom derivative (F_{ph}) is ambiguous (more than one possible choice of phase value). Describe two different types/sources of phase ambiguity in the SIR (single isomorphous replacement) experiments, and at least two methods (experimental or computational) to identify the correct phase value.

8. Give 2 reasons why the rotation function for molecular replacement is typically calculated at low resolution ($10 - 4 \text{ \AA}$) instead of over the full resolution range of the x-ray data for the unknown crystal. For an unknown crystal with multiple protein molecules in the asymmetric unit, does limiting the resolution improve the odds of obtaining a correct rotation solution using a single protein?