MSE 102, Fall 2011 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

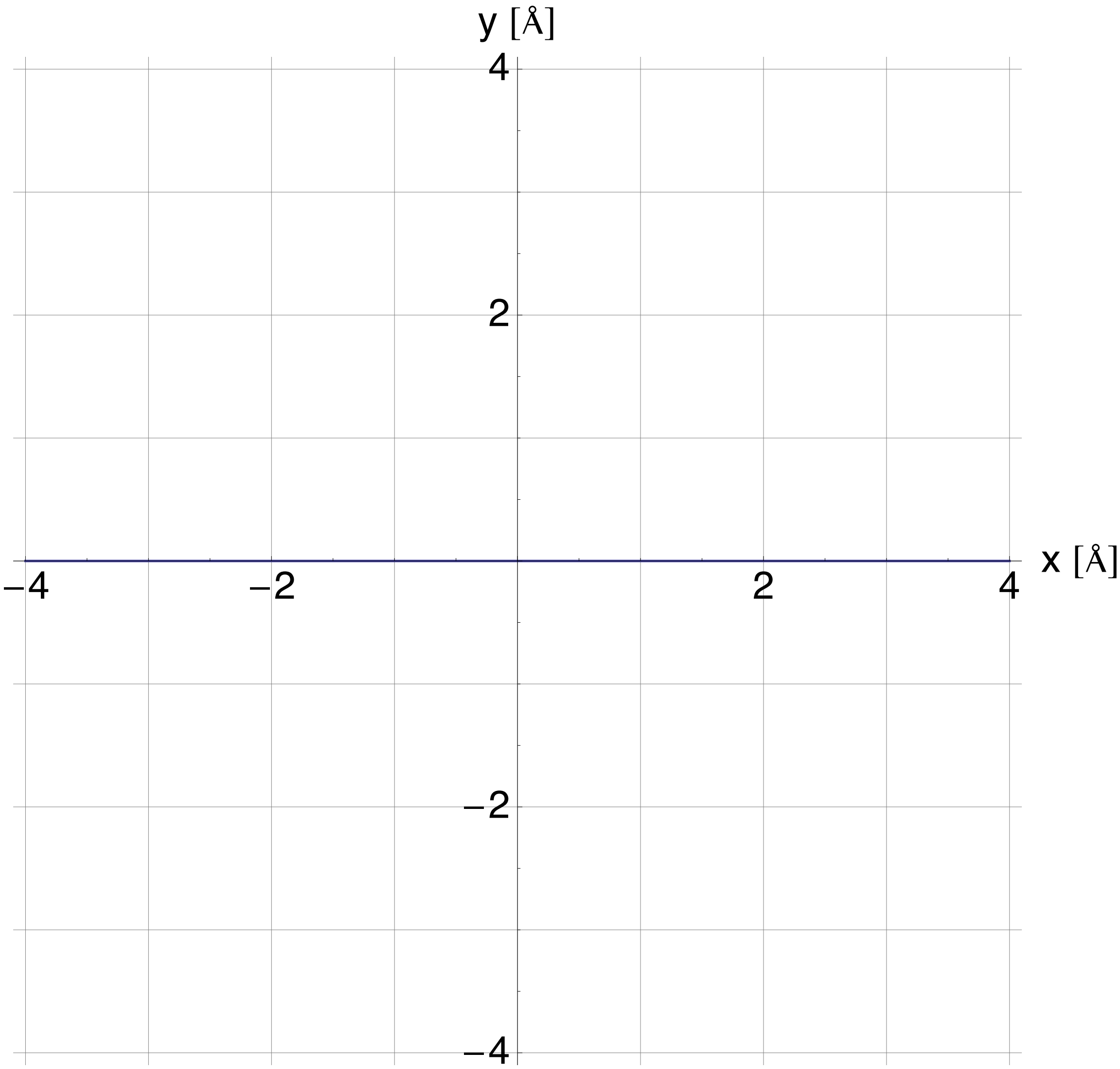
Problem 1. A 2-D crystal has an atomic scale structure described by the symmetry group *p4gm* (see the attached entry from the International Tables for Crystallography). The lattice parameter (i.e. the length of the vector **a**) is equal to 2 Å. There are Si atoms at Wyckoff position(s) *d*.

Carry out the following instructions:

1. (5 points) On the attached graph, plot the positions of the lattice points with an ×. Plot all of the lattice points that appear in the range of the plot.

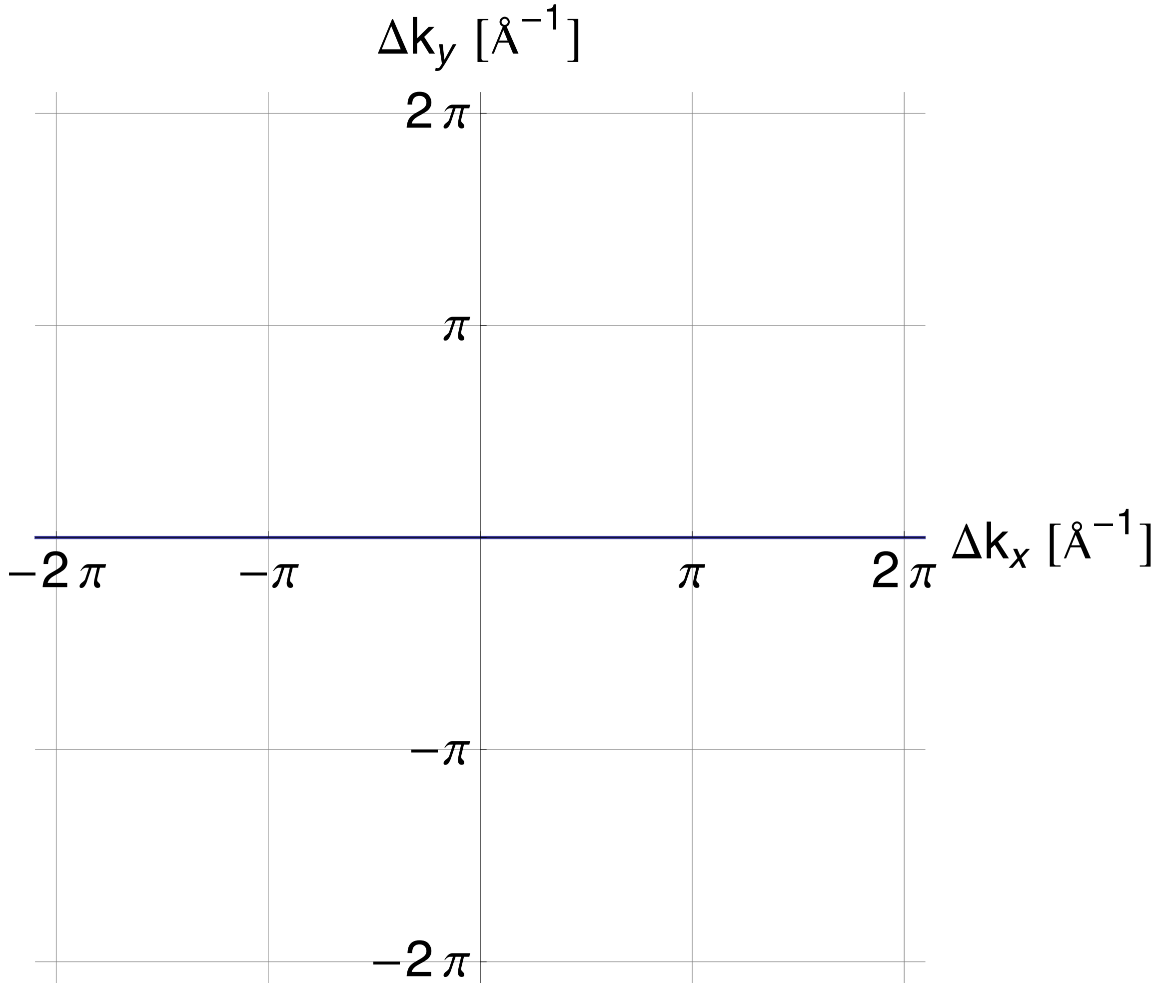
2. (5 points) Identify a set of primitive lattice vectors for the crystal. Write their coordinates here (in terms of $\mathbf{e_x}$ and $\mathbf{e_y}$) and draw them on your plot of the lattice.

3. (5 points) Identify the Wigner-Seitz cell for this crystal on your plot. (5 points) How many atoms are there per unit cell? (5 points) Is the unit cell primitive?


y [Å]
4
2
−2
−4
x [Å]
−4
−2
2
4

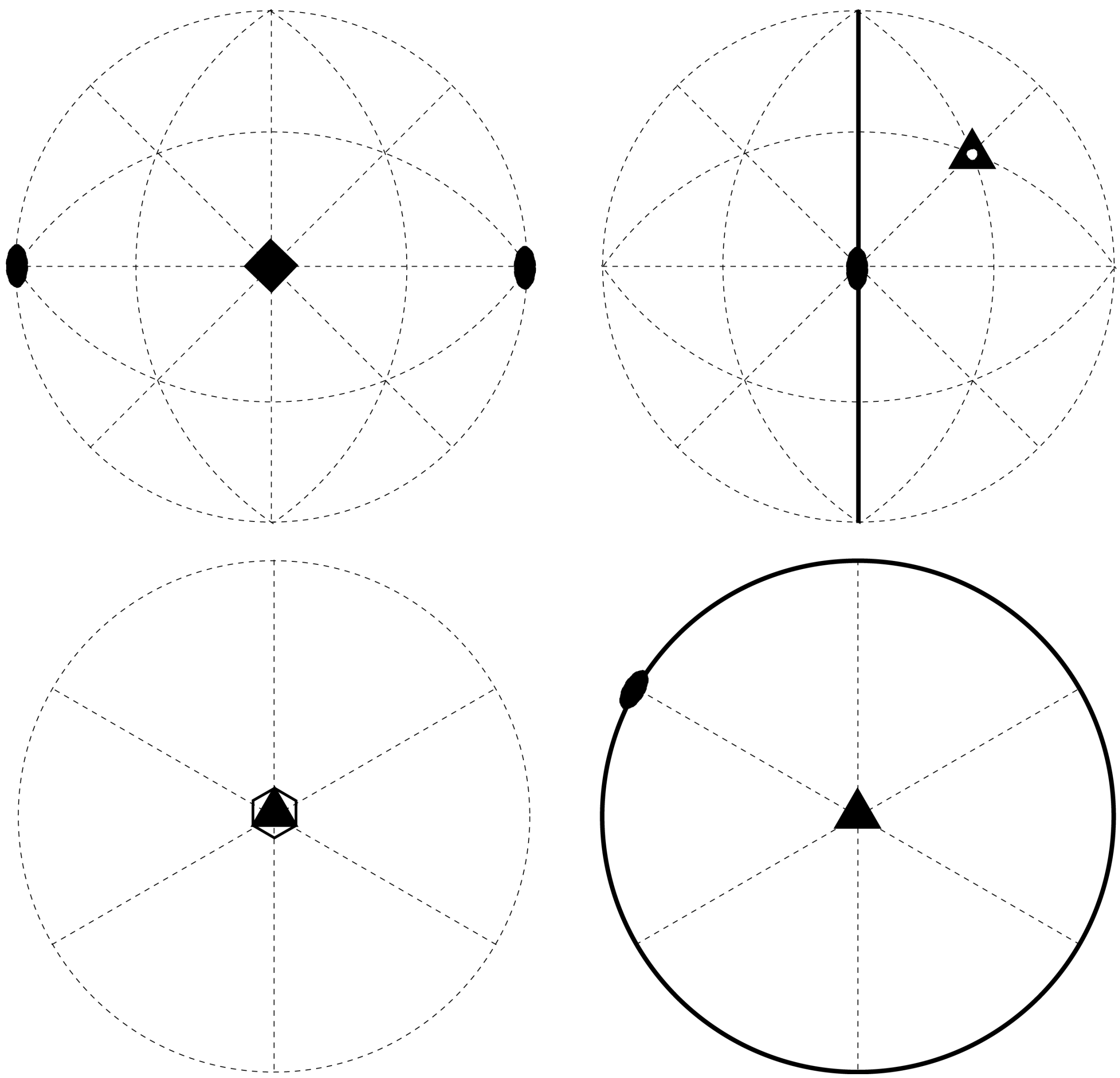
4. (5 points) Construct the primitive reciprocal lattice vectors for this crystal and write them in terms of $\mathbf{e}_x$ and $\mathbf{e}_y$. On the graph below sketch the vectors and plot the positions of the reciprocal lattice points by marking them with an $\times$. Indicate the positions of all reciprocal lattice vectors in the range of the plot.

5. (5 points) On the same plot, indicate with an $\circ$ the points at which you expect to see diffraction peaks based on the conditions given in the Plane Group table entry. (That is, don't worry about additional effects associated with the fact that x and y may have specific values.)

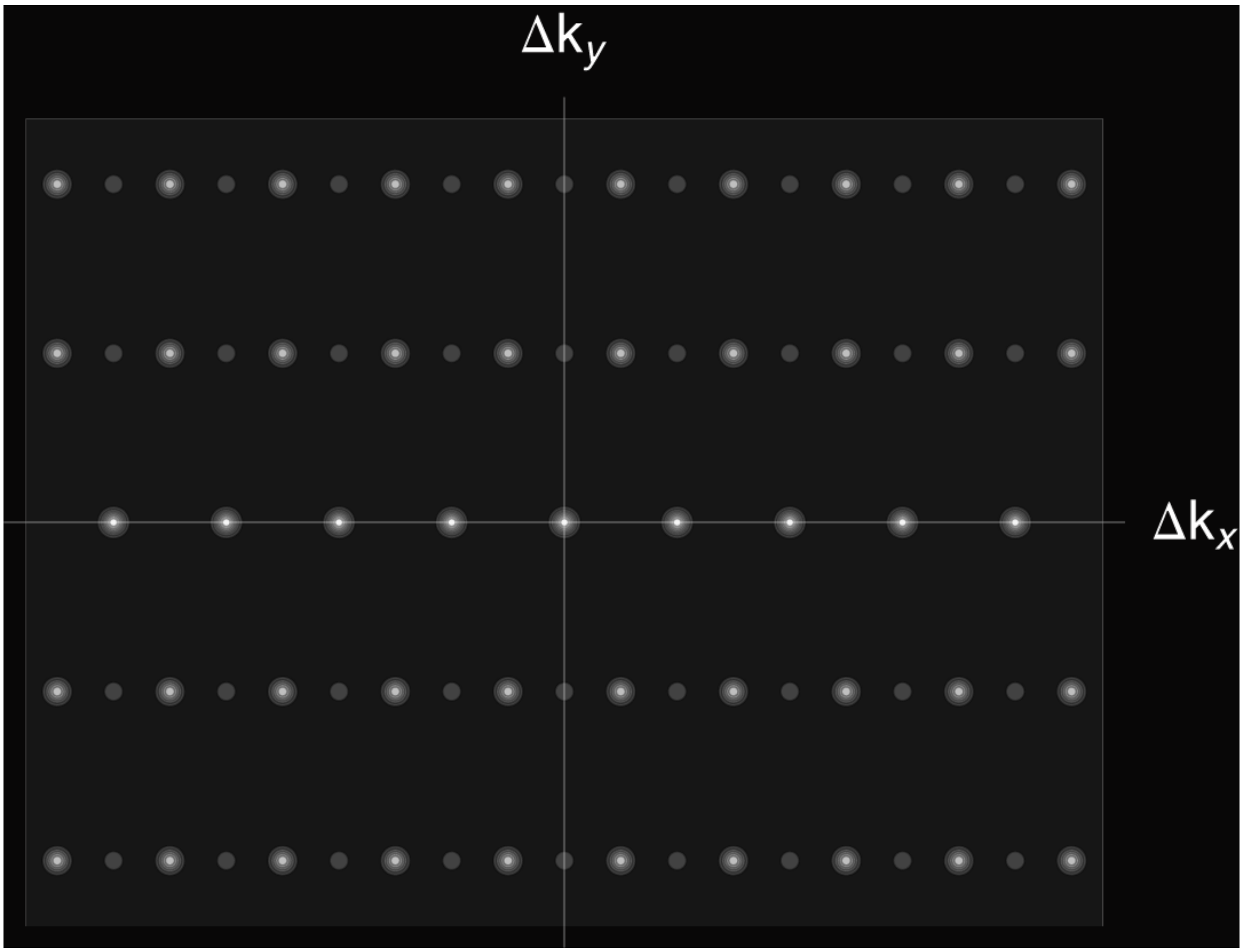


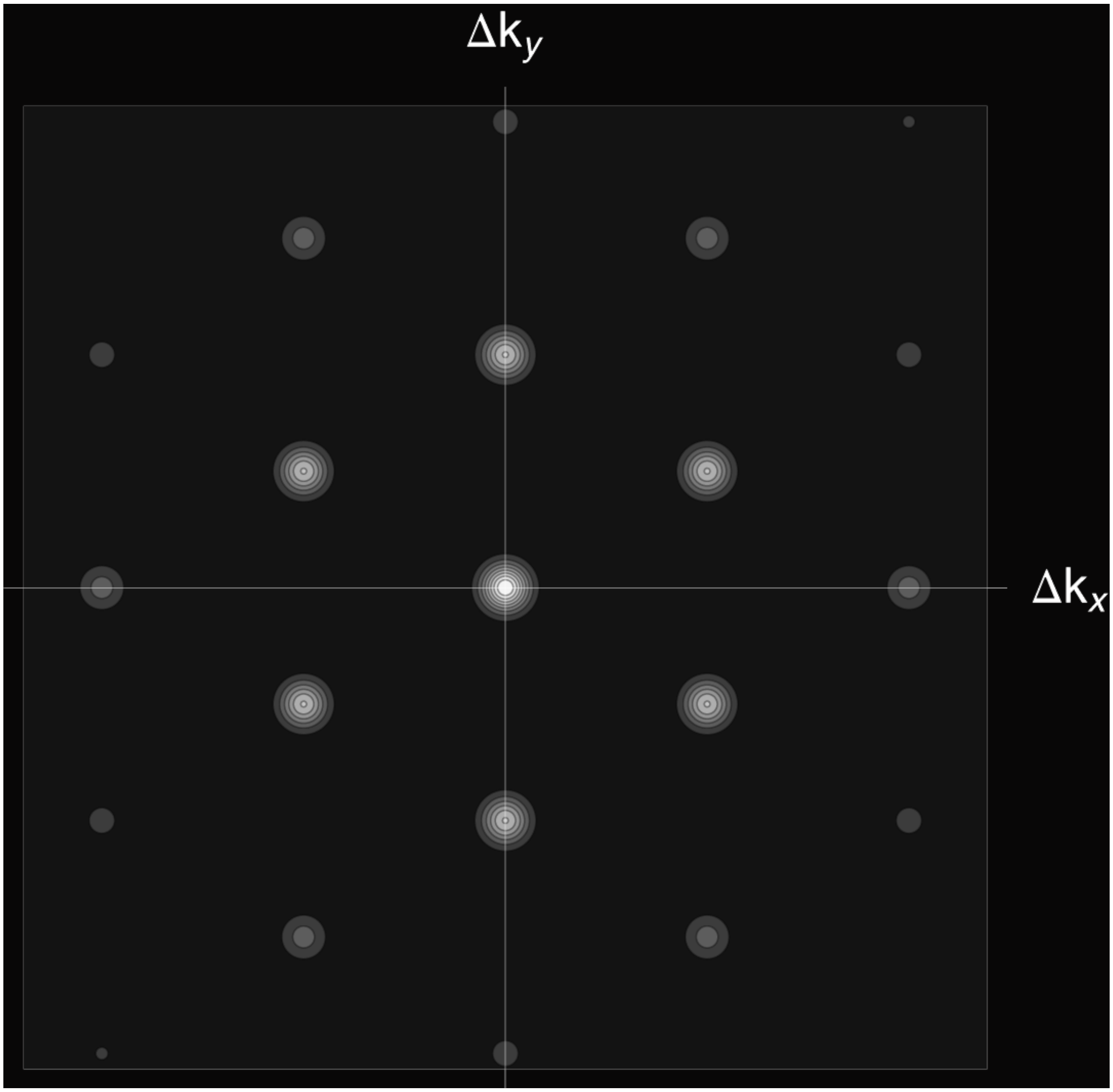
Δk_y [$\AA^{-1}$]
2π
π
$-\pi$
-2π
Δk_x [$\AA^{-1}$]
-2π
$-\pi$
π
2π

Problem 2. (5 points each) Complete the following stereograms. Indicate all symmetry elements on the stereogram (no need to list them explicitly), and which directions are equivalent by symmetry. Be sure to pick a direction that does *not* lie on a symmetry element. [You will lose one point per incorrect (either missed or erroneously present) symmetry operation and equivalent direction (up to the maximum value of each stereogram).]

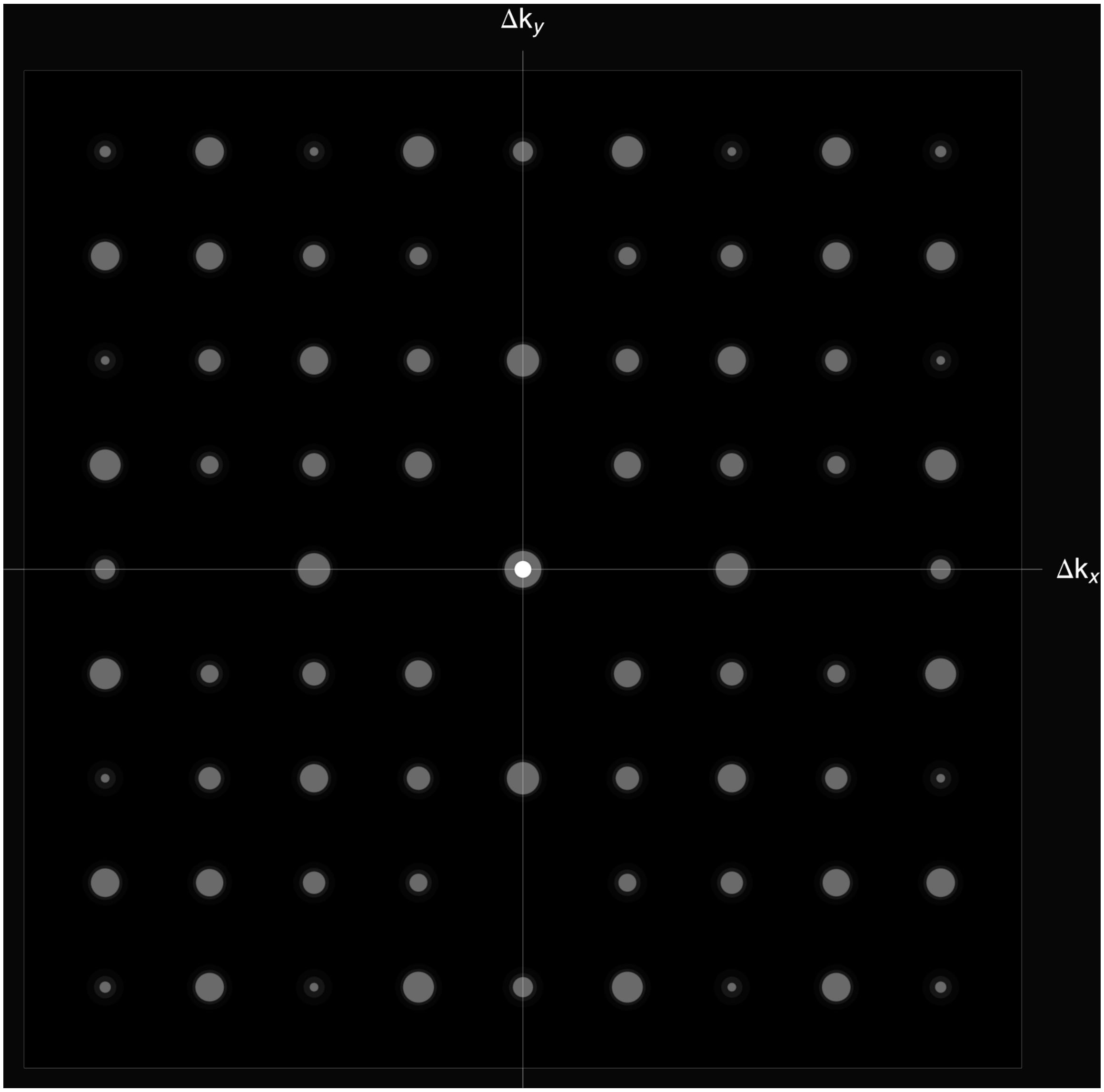


Problem 3. The following patterns are calculated diffraction patterns for 2D crystals. The size and brightness of the spot corresponds to the intensity. (2 points each) Based on these diffraction patterns, identify the plane group (or plane groups) that might describe the symmetry of the crystal. (3 points each) Give a brief but clear justification for each of your answers.





Δk_y
Δk_x


Δk$_y$
Δk$_x$

Problem 4. The primitive lattice vectors of a 2D crystal are given by:

$$\mathbf{a} = -\frac{1}{2}\mathbf{e}_x - \frac{\sqrt{3}}{2}\mathbf{e}_y$$
$$\mathbf{b} = 1\mathbf{e}_x$$

(5 points) Find the primitive reciprocal lattice vectors for this lattice. Express them in terms of $\mathbf{e_x}$ and $\mathbf{e_y}$. (5 points) Sketch the lattice vectors and reciprocal lattice vectors using the same origin and coordinate system.

Problem 5. The image below is an atomic scale sketch of a portion of a known 2-D crystal.

(a) (5 points) Identify the lattice points in the sketch. Mark them with an $\times$. (You only need to identify enough of the points to prove that you have identified the lattice.)

(b) (5 points) Identify a primitive unit cell. How many atoms are in a primitive unit cell? Sketch the basis vector for each atom in the primitive unit cell.

(c) (5 points) Sketch all of the symmetry operations in the primitive unit cell you sketched above. Include those (if any) on the boundary of the cell. Give the name of the plane group describing the symmetry of this crystal.

(d) (5 points) Identify the asymmetric unit for the crystal.