Problem 1:
For each of the following lattices:

a) give two primitive vectors and draw them
b) draw a primitive cell, c) list all the point group
symmetries of the lattice, d) indicate the Bravais lattice type

i) 

\[ \hat{a}_1 = a(1, 0) \]
\[ \hat{a}_2 = a \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \]

\[ c) \ 2\pi, \ \pi, \ \frac{\pi}{3}, \ \frac{2\pi}{3}, \ \text{mirror} \]
\[ d) \ \text{hexagonal/triangular} \]

ii) 

\[ \hat{a}_1 = a(1, 0) \]
\[ \hat{a}_2 = a(0, 1) \]

\[ c) \ 2\pi, \ \pi, \ \frac{\pi}{4}, \ \text{mirror} \]
\[ d) \ \text{square} \]

iii) 

\[ \hat{a}_1 = a(1, 0) \]
\[ \hat{a}_2 = b(0, 1) \]

\[ c) \ 2\pi, \ \pi, \ \text{mirror} \]
\[ d) \ \text{rectangular} \]

iv) 

\[ \hat{a}_1 = a(1, 0) \]
\[ \hat{a}_2 = \left( \frac{a}{2}, \frac{b}{2} \right) \]

\[ c) \ 2\pi, \ \pi, \ \text{mirror} \]
\[ d) \ \text{centered rectangular} \]
Problem Set 1

#2

Braun's Lattice

\[ \hat{a}_1 = \sqrt{3}a(0, -1) \]

\[ \hat{a}_2 = \sqrt{3}a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \]

Note: this is a hexagonal/triangular B.L.

\[ \frac{\sqrt{3}}{2}a = \sqrt{3}a \]

\[ \frac{3a}{2} \]

basis = B.L. + \(-\frac{1}{2}a(1, 0) + \frac{1}{2}a(1, 0)\)

area of prim cell: 

\[ A = \frac{1}{2} |\hat{a}_1 \times \hat{a}_2| \]

\[ = (\sqrt{3}a)^2 \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & -1 & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \end{vmatrix} \]

\[ = 3a^2 (1 + \frac{\sqrt{3}}{2}) = \frac{3\sqrt{3}}{2}a^2 \]

Note: this is the area of hexagon w/side a
Problem 3

For all 3 lattices assume a cubic conventional cell w/ lattice vectors:

\[ \vec{a}_1 = a \hat{x} \quad \vec{a}_2 = a \hat{y} \quad \vec{a}_3 = a \hat{z} \]

(a) Base-centered is a **Braun's lattice** (tetragonal)

A set of primitive lattice vectors is:

\[ \vec{a}_1 = a \frac{1}{2}(\hat{x} + \hat{y}) \]
\[ \vec{a}_2 = a \frac{1}{2}(\hat{x} - \hat{y}) \]
\[ \vec{a}_3 = a \hat{z} \]

Volume: \( V_c = a^3 / 2 \)

b) Side-centered is **NOT** a Braun's lattice

to see this, note that we can construct 3 vectors that generate all points on the lattice, i.e.

\[ \vec{a}_1 = a \frac{1}{2}(\hat{x} + \hat{z}) \]
\[ \vec{a}_2 = a \frac{1}{2}(\hat{y} + \hat{z}) \]
\[ \vec{a}_3 = a \hat{z} \]

### but these vectors also

generate "extra" points not on the lattice. i.e. \( \vec{a}_1 + \vec{a}_2 \)

Also, note that the array of points has a different appearance viewed from \( A \ leq B \).

This lattice is a simple cubic + a \( 3 \)-atom basis at

basis = \( (0,0,0) + (1/2,0,1/2) + (0,1/2,1/2) \)
3c  Edge-centered cubic is NOT a B.L.
again \( \mathbf{a}_1 = \frac{a}{2} \hat{x} \), \( \mathbf{a}_2 = \frac{a}{2} \hat{y} \), \( \mathbf{a}_3 = \frac{a}{2} \hat{z} \)
generate the lattice, but their sum is not a lattice point:
\( \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 \notin \text{ECC} \)
the lattice is a simple cubic with a 4-atom basis
\((0,0,0) + (\frac{a}{2},0,0) + (0,\frac{a}{2},0) + (0,0,\frac{a}{2})\)

4) Diamond structure:

a) \( \text{fcc} + 2 \) point basis at \((0,0,0)\) and \( \frac{a}{4} (\hat{x} + \hat{y} + \hat{z}) \)
4 not shared
8 at corners \( \left( \frac{a}{2} \right) = 1 \)
6 at faces \( \left( \frac{a}{2} \right) = 3 \)

\( \text{this crystal has 8 atoms in the conventional cell.} \)
\[ V_{PC} = a^3 / 8 \]

b) \[ \phi = \frac{8 \cdot V_S}{V_C} \]
\[ V_C = a^3 \text{ and } V_S = \frac{4}{3} \pi r^3 \]

What is the max sphere radius at close packing?
distance from one basis atom to the other is
\[ d = \frac{\sqrt{3} a}{4} = 2r \]
4 b) cont'd

so \( r = \frac{\sqrt{3} a}{8} \)

\[
\Phi_{cp} = 8 \cdot \frac{4/3 \pi \left(\frac{\sqrt{3}}{8}\right)^3 a^3}{a^3}
\]

\[
= \frac{\sqrt{3} \pi}{16} \approx 0.34
\]

This is very low

-> diamond structure is very inefficient compared to fcc.

5: HCP structure

\( a \)

So let \( a(\frac{1}{2}, \sqrt{3}/2) \)

Layer A be \( (0, 0) \) \( (a, 0) \) \( a \) standard triangular lattice.

B: what are these coordinates? (equidistant from layer A points)

\[
|\mathbf{B}_{xy} - (0, 0)| = |\mathbf{B}_{xy} - (a, 0)| = |\mathbf{B}_{xy} - (\frac{1}{2}, \sqrt{3}/2)|
\]

\[
\Rightarrow \frac{1}{4} + b^2 = (\frac{\sqrt{3}}{2} - b)^2 \Rightarrow 0 = \frac{1}{2} - \sqrt{3}b \Rightarrow b = \frac{1}{2\sqrt{3}}
\]

\[
\mathbf{B}_{xy} = a(\frac{1}{2}, \frac{1}{2\sqrt{3}})
\]
5a) cont'd

the z-coord of B is \( \frac{1}{2} c \).

Then at close packing, we know the distance b/w A & B layers particles should be \( d = a \)

\[
d = \left| \vec{B} - (0, 0, 0) \right|
\]

\[
= \sqrt{x^2 - 0^2 + (y - 0)^2 + (z - 0)^2}
\]

\[
d = a \sqrt{\frac{1}{4} a^2 + \frac{1}{12} a^2 + \frac{1}{12} c^2}
\]

Want this to be the same distance b/w particles in layer A

\[
a^2 = \frac{1}{4} a^2 + \frac{1}{12} a^2 + \frac{1}{4} c^2
\]

\[
\Rightarrow \frac{12 \cdot 3 \cdot 1}{12} a^2 = \frac{1}{4} c^2 \Rightarrow \frac{2 \cdot 4}{3} a^2 = c^2
\]

\[
\Rightarrow c = \sqrt{\frac{8}{3}}a
\]

b) Packing fraction:

\[2r = d\] at close packing

What is HCP? Not a Bravais lattice;

it is a simple hexagonal B.L w/ a two-point basis:

\[
\phi = 2 \cdot \frac{4/3 \pi (a/2)^3}{V_{p.c.}}
\]

\[\Rightarrow 2\text{ spheres in each primitive cell}\]
5b) cont'd:

primitive vectors are
\[
\hat{a}_1 = a \hat{x} \\
\hat{a}_2 = \frac{a}{2} \hat{x} + \frac{\sqrt{3}a}{2} \hat{y} \\
\hat{a}_3 = c \hat{z}
\]

\[\Rightarrow V_{pc} = \left| \hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3) \right| \]

\[= a^3 \left| \begin{array}{ccc}
1 & 0 & 0 \\
\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\
0 & 0 & \sqrt{3}
\end{array} \right| = \sqrt{2} a^3 \]

\[\Rightarrow \phi = \frac{\pi}{3\sqrt{2}} \approx 0.704 \text{ same as fcc. } \]