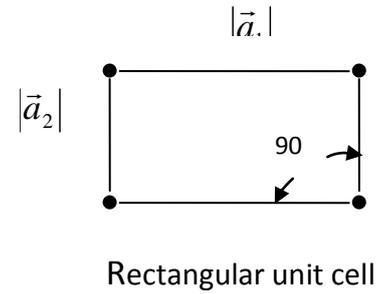


1) The diagram shows the conventional unit cell of a rectangular lattice (sides a_1 and a_2).

- Write down the fractional co-ordinates of all the lattice points.
- Write down suitable primitive lattice vectors.
- Calculate the area of a primitive unit cell.
- Sketch the Wigner Seitz cell for this lattice.
- What is the maximum packing fraction?

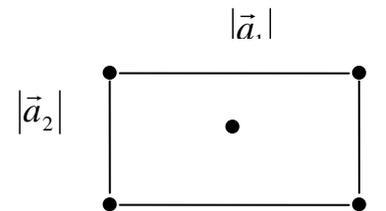
[Hint for (v): first work out the maximum radius of circles which just touch one another when placed at nearest neighbour sites; then compare the area of such a circle with that of the primitive unit cell].



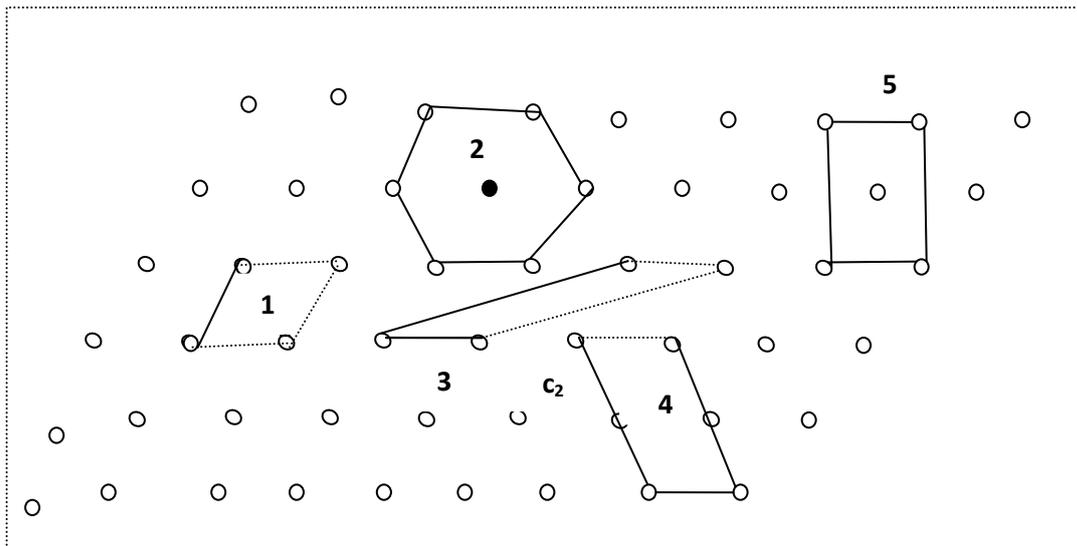
Rectangular unit cell

2) Repeat question (1) for a centered rectangular lattice.

[N.B. the primitive lattice vectors are not the same and still there must be only one lattice point per primitive unit cell].



- The diagram shows a portion of a 2D lattice. Which of the outlines represent
 - primitive unit cells,
 - non-primitive unit cells;
 - not unit cells at all



4) Prove that the ideal ratio of c/a for a hexagonal close packed structure is 1.633.

5) What is the coordination number for a bcc lattice with a one-atom basis? Show that the packing fraction for identical hard spheres arranged in a bcc lattice is 0.680.

6) For the fcc lattice with a one atom basis:

- (i) what is the co-ordination number?
- (ii) how many second-nearest-neighbours does each atom have?
- (iii) what is the distance to these, in units of the conventional cubic lattice side a ?
- (iv) what is the separation between close-packed planes? Answer: Close packed planes are (111) with spacing $a/\sqrt{3}$.

7) At 1190 K, iron has a cubic-F (fcc) lattice with cube edge 0.3647 nm, while at 1670 K it has a cubic-I (bcc) lattice with cube edge 0.2932 nm. In both cases there is a one-atom basis. Calculate the ratio of the densities of iron at these two temperatures. Answer :Ratio of densities is 0.962.

8) A 2D direct lattice has primitive lattice vectors: $\vec{a}_1 = a_1 \hat{x}$, $\vec{a}_2 = a_2 ((\cos\theta)\hat{x} + (\sin\theta)\hat{y})$

[Note: these are just vectors of magnitudes a_1 and a_2 with angle θ between them].

a) Sketch a portion of this lattice, indicating the cartesian axes and the primitive lattice vectors

b) Show that the reciprocal lattice has primitive vectors: $\vec{b}_1 = \frac{2\pi}{a_1} (\hat{x} - \frac{\cos\theta}{\sin\theta} \hat{y})$,

$$\vec{b}_2 = \frac{2\pi}{a_2} (\frac{1}{\sin\theta} \hat{y}).$$

[Note: the 2D reciprocal lattice can be determined in two ways:

EITHER: write \vec{b}_1 and \vec{b}_2 as general vectors in 2D and then determine the values of their x and y components that allow them to satisfy the Laue condition;

OR: use the formulae relating 3D reciprocal and direct lattice vectors, but use $\vec{a}_3 = a_3 \hat{z}$ for the third direct lattice vector and allow a_3 to tend to infinity. The third reciprocal lattice vector will then be of magnitude zero, and can simply be ignored.]

c) Sketch the reciprocal lattice indicating its orientation with respect to the direct lattice. [Hint: you should find that \vec{b}_1 is perpendicular to \vec{a}_2 and \vec{b}_2 is perpendicular to \vec{a}_1]

d) Sketch both the direct and reciprocal lattices in the case $a_1 = 0.1$ nm, $a_2 = 0.2$ nm, $\theta = 60^\circ$. [Hint: they should be rectangular.]

e) On your sketch of the rectangular reciprocal lattice above, construct the first and second Brillouin zones. [Note: you know how to construct the first one. The second Brillouin zone is the region of k -space (not necessarily a single region) reached from the chosen reciprocal lattice point, by crossing one, and only one, perpendicular bisector – it should have the same 'volume' as the first Brillouin zone.