Assessment
Solid-state physics

UNIVERSITY of TASMANIA

Assignment 4: Crystals

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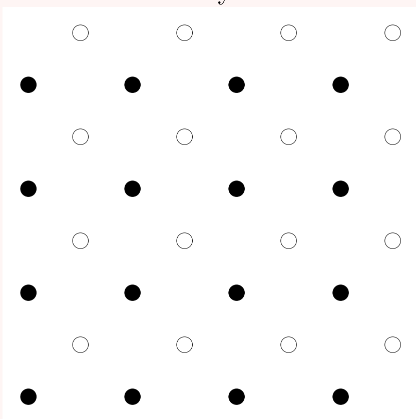
Due: 1700, October 04, 2021

Exercise 1 *Two-dimensional crystal structure* (9 points)

Consider the following two-dimensional diatomic crystal:

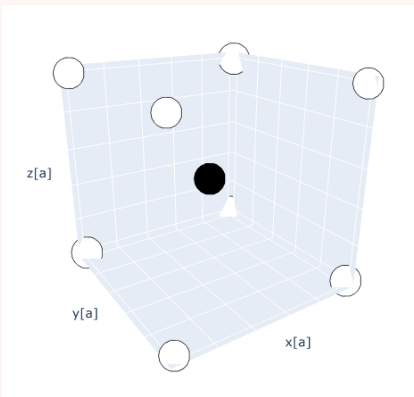


(i) Sketch the Wigner-Seitz unit cell and two other possible primitive unit cells of the crystal

(ii) If the distance between the filled circles is $a = 2.8\,\text{Å}$, what is the area of the primitive unit cell? How would this area change if all the empty circles and the filled circles were identical?

(iii) Write down one set of primitive lattice vectors and the basis for this crystal. What happens to the number of elements in the basis if all empty and filled circles were identical?

(iv) Imagine expanding the lattice into the perpendicular direction z. We can define a new three-dimensional crystal by considering a periodic structure in the z direction, where the filled circles have been displaced by $\frac{a}{2}$ in both the x and y direction from the empty circles. The figure below shows the new arrangement of the atoms.

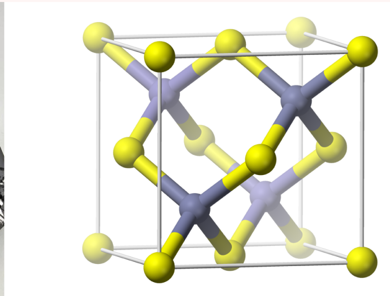


What lattice do we obtain? Write down the basis of the three-dimensional crystal.

(v) If we consider all atoms to be the same, what lattice do we obtain?

Exercise 2 *Three-dimensional crystal structure* (6 points)

The image below shows the three dimensional structure of zincblende (ZnS) (zinc atoms are yellow, sulphur atoms are grey).



(i) How many atoms are in the unit cell?

(ii) Draw the plan view of the unit cell

(iii) Identify the lattice type of zincblende

(iv) Describe the basis for zincblende

(v) Given the unit cell length $a = 5.41\,\text{Å}$, calculate the nearest-neighbour Zn-Zn, Zn-S, and S-S distances

Exercise 3 *Filing factor* (6 points)

Consider a lattice with a sphere at each lattice point, and choose the radius of the spheres to be such that neighbouring spheres just touch. The filling factor (or packing fraction) is the fraction of the volume of all of space which is enclosed by the union of all the spheres (i.e. the ratio of the volume of the spheres to the total volume).

(i) Calculate the packing fraction for a simple cubic lattice

(ii) Calculate the packing fraction for a BCC lattice

(iii) Calculate the packing fraction for an FCC lattice

Exercise 4 *Reciprocal lattice* (6 points)

(i) Show that the reciprocal lattice of a FCC lattice is a BCC lattice. Correspondingly, show that the reciprocal lattice of a BCC lattice is an FCC lattice

(ii) If an FCC lattice has conventional unit cell with lattice constant a, what is the lattice constant for the conventional unit cell of the reciprocal BCC lattice?

(iii) Consider now an orthorhombic face-centred lattice with conventional lattice constants a_1, a_2, a_3. What is the reciprocal lattice now?