

**Exercise 1: Crystal structure**

1. a) Calculate the packing fraction of face-centered cubic (FCC) crystal structure by assuming that the atoms are hard spheres with a radius of  $R$  (all the same size). Then calculate the relative volume that the spheres take for themselves, if the nearest neighbour spheres are touching each other. b) Calculate the volume of the unit cell starting from the primitive vectors shown in the lecture.
2. a) Calculate the packing fraction for diamond/zinc-blende crystal structure as described in problem 1. b) Calculate the angle  $\alpha$  between the tetrahedral bonds.
3. a) Calculate the packing fraction for hexagonal close packed (HCP) crystal structure lattice. The structure (in the figure) consists of tetrahedrons with equilateral side triangles (the length of all the sides is equal). b) Calculate the ideal ratio  $c/a$  for the HCP structure ( $a$  = lattice constant in the hexagonal plane,  $c$  = distance of the upper and lower planes in the figure).
4. Gallium nitride (GaN) crystallizes most probably in wurtzite crystal structure, although zinc blende GaN is also possible. Calculate the density of wurtzite GaN. The lattice constants of GaN are  $a = 3.186 \text{ \AA}$ ,  $c = 5.186 \text{ \AA}$  and the atomic mass of GaN is 83.73 amu.

