

1. Consider a crystal made up of one atom per lattice site for each of the three cubic Bravais lattices, simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc).
 - (a) Sketch the structures.
 - (b) In each case, determine how many nearest neighbors each atom has (the coordination number)?
 - (c) Find how many atoms are there per conventional unit cell (cube), and thus determine the volume of a primitive unit cell compared to the conventional unit cell?
 - (d) If the side of the cube has length a , determine the spacing between nearest neighbors?
 - (e) Determine the packing fraction, i.e., the maximum fractional volume that can be filled by non-overlapping solid spheres.
2.
 - (a) Repeat problem 2 for the diamond structure (fcc with a two atom basis such that for each lattice site (x,y,z) there is an atom at (x,y,z) and another at $(x+1/4, y+1/4, z+1/4)$).
 - (b) Find the nearest neighbor distance for the diamond phase of carbon, silicon and germanium, given their densities are 3.515, 2.329, 5.323 g/cm³ respectively.
 - (c) In the diamond structure, each atom makes a covalent bond with each of its nearest neighbors (you should have found four). Find the angle between these tetrahedral bonds?
3. In 1986, Bednorz and Müller first reported on the possibility of high-temperature superconductivity in the La-Ba-Cu-O system, setting off a renewed interest in the field of superconductivity and for which they would later share the Nobel prize. The underlying host structure turned out to be a La₂CuO₄ that when doped with a little Ba forms a centered tetragonal structure.

Look up the primitive and basis vectors for this structure at (click on the link or type into your browser) <http://cst-www.nrl.navy.mil/lattice/struk/hightc/x0201.html>

Important for superconductivity is the Cu-O(I) planes perpendicular to the tetragonal (z) axis. Sketch a single one of these layers and show that it forms a 2D Bravais lattice by indicating the primitive lattice vectors and a primitive unit cell. Notice the oxygen forms along diagonal lines in the (x - z) plane. The actual structure is slightly distorted with every other line is raised/lowered slightly out of the plane. Does this change the unit cell? If so how?
4.
 - (a) Show that the c/a ratio for an ideal hexagonal close-packed structure is $\sqrt{8/3}$.
 - (b) Solid sodium transforms from bcc to hcp at about 23K. The lattice constant in the cubic phase is 4.23 Å. Find the lattice constant of the hexagonal phase, assuming that the density remains fixed in this phase transition (martensitic).