PHYS 558 Solid State Physics
Assignment 1: Crystal Structures

Due on: 2022 Sept. 15 (Thursday, on Crowdmark before 17:00)

1. **Packing fraction (A+M 4.6)**
   The face-centered cubic is the most dense and the simple cubic is the least dense of the cubic Bravais lattices. The diamond structure is less dense than any of these. One measure of this is that the coordination numbers are: fcc, 12; bcc, 8; sc, 6; diamond, 4. Another is the following: Suppose identical solid spheres are distributed through space in such a way that their centres lie on the points of each of these four structures, and spheres on neighbouring points just touch, without overlapping. This is called a close-packed arrangement. Assuming that the spheres have unit density, show that the density of a set of close-packed spheres on each of the four structures (the "packing fraction") is:

   (a) fcc: $\sqrt{2}\pi/6 = 0.74$
   (b) bcc: $\sqrt{3}\pi/8 = 0.68$
   (c) sc: $\pi/6 = 0.52$
   (d) diamond: $\sqrt{3}\pi/16 = 0.34$.

2. **Wigner-Seitz cell**
   On a piece of graph paper (by hand) or by using plotting software, draw:

   (a) a few (say, 5×5) cells of a rectangular lattice having primitive lattice translations $\mathbf{a}_1 = a\hat{x}$, $\mathbf{a}_2 = b\hat{y}$, with $a/b = 3/2$. Construct a Wigner-Seitz cell near the centre of your array (you can do this either by hand using a ruler and protractor or using plotting software, but hand in the input file used if you do this in software).
   (b) Now do the same for a two-dimensional hexagonal (triangular) lattice.

3. **Reciprocal lattice (A+M 5.2)**

   (a) Show that the reciprocal of the (3D) simple hexagonal Bravais lattice is also simple hexagonal with lattice constants $2\pi/c$ and $4\pi/\sqrt{3}a$, rotated by 30° about the c-axis relative to the direct lattice.
   (b) For what value of c/a does the ratio have the same value in both the direct and reciprocal lattices? If c/a is ideal in the direct lattice, what is its value in the reciprocal lattice?
   (c) The Bravais lattice generated by three primitive vectors of equal length a, making equal angles θ with one another, is known as the trigonal Bravais lattice (see Chapter 7 in A+M). Show that the reciprocal of a trigonal Bravais lattice is also trigonal, with an angle θ^* given by $-\cos\theta^* = \cos\theta / [1 + \cos\theta]$, and a primitive vector of length a^*, given by $a^* = (2\pi/a)(1 + 2\cos\theta\cos\theta^*)^{-1/2}$.

4. **Stacked hexagonal lattices**
   Calculate the scattering intensity for the following close-packed structures formed by stacks of hexagonal lattices:

   (a) The sequence $ABAB\cdots$ (the hcp structure)
   (b) The sequence $ABCABC\cdots$. Show that scattering from this surface is that of an fcc lattice.