1. The simple cubic (SC) lattice with lattice parameter $a$ can be defined by three basis vectors:

\[ \mathbf{a}_1 = a(1,0,0) \quad \mathbf{a}_2 = a(0,1,0) \quad \mathbf{a}_3 = a(0,0,1) \]

Obviously, $|\mathbf{a}_1| = |\mathbf{a}_2| = |\mathbf{a}_3|$, and the angles between the basis vectors are all 90 degrees. These vectors are defined by connecting the origin $(0,0,0)$ to three nearest-neighbor lattice points: (100), (010) and (001).

In class we considered the body-centered cubic (BCC) lattice as a cubic lattice with the same base vectors but two atoms per unit cell (at $(0,0,0)$ and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$). However, the BCC lattice can also be defined by the basis vectors:

\[ \mathbf{a}_1 = a(-\frac{1}{2},\frac{1}{2},\frac{1}{2}) \quad \mathbf{a}_2 = a(\frac{1}{2},-\frac{1}{2},\frac{1}{2}) \quad \mathbf{a}_3 = a(\frac{1}{2},\frac{1}{2},-\frac{1}{2}) \]

by connecting the origin $(0,0,0)$ to its nearest neighbor points. Such a cell contains exactly one atom per unit cell, and is known as a **primitive unit cell**.

   a. Show that for this primitive unit cell $|\mathbf{a}_1| = |\mathbf{a}_2| = |\mathbf{a}_3|$. Compute $|\mathbf{a}| (=|\mathbf{a}_1|=|\mathbf{a}_2|=|\mathbf{a}_3|)$ in terms of $a$, and compute the angles between the basis vectors using vector analysis.

   b. Compute the volume of the BCC primitive unit cell, and show that this is consistent with considering the BCC unit cell as a cube of dimension $a$ with two atoms per unit cell.

2. The reciprocal lattice of the simple cubic lattice is itself a cubic lattice, with the reciprocal lattice parameter $b = \frac{2\pi}{a}$. This can be shown using Eq. (13) on p. 29 of Kittel.

Show that the reciprocal lattice of the BCC primitive lattice (using the definition in Problem 1) is a primitive FCC lattice, using vector analysis. (The reverse is also true: the reciprocal lattice of FCC is BCC.)

3. Show that the structure factor for a reflection $(hkl)$ from the FCC lattice is zero unless $h$, $k$ and $l$ are all even or all odd.

4. (a) I’m doing an x-ray diffraction experiment on metallic aluminum. Compute the Bragg angles $(2\theta)$ of the first three nonzero reflections, if I’m using a Cu Kα x-ray source ($\lambda = 1.541$ Å). (Cu is probably the most widely-used x-ray source due to long life, reasonable operating voltage, and a wavelength which is ideally suited for “general purpose” diffraction measurements.

   (b) I replace the Cu source with a Mo source ($\lambda = 0.7107$ Å). How would this affect the produced x-ray pattern, and what would be the pros and cons of using such a source?

   (c) Now I replace the source with a Cr tube ($\lambda = 2.290$ Å). How does this affect the diffraction pattern, and what would be the pros and cons of using this tube (relative to Cu)?
Neutrons are produced at a reactor or spallation source via high-energy nuclear reactions. These neutrons typically have energies on the order of MeV (mega electron volts). These energies are way too high to be of use for diffraction experiments. So, the neutrons are passed through a moderator (typically water at room temperature, 300K), and, after repeatedly scattering off of atoms or molecules in the moderator, the neutrons achieve thermal equilibrium with the moderator. This means that the energies and velocities of neutrons produced follow a Maxwellian distribution with a most probable energy $E = k_B T$, where $T$ is the temperature of the moderator, and $k_B$ is Boltzmann’s constant. (The average energy is $\frac{3}{2} k_B T$, because it is a skewed distribution, but the most probable value – the peak of the distribution where the greatest number of neutrons are produced – is at $k_B T$.)

a. What is the most probable energy $E$ of these “thermal” neutrons?
b. What wavelength do these neutrons have? (Hint: the neutrons have low enough energy to be non-relativistic, and the wavelength is the de Broglie wavelength $\lambda = h/p$.)
c. How does this wavelength compare to that of the interatomic spacings in a crystal?