(1)     A 3-dimensional tetragonal crystal has an energy band as follows:

$$\varepsilon(k) = \frac{\hbar^2}{2m_1}\left(k_x^2 + k_y^2\right) + \frac{\hbar^2}{2m_2}k_z^2,$$                                   [1]

where $m_1$ and $m_2$ are constants, and for this crystal, $m_2 = 4\,m_1$.

(a) If this band is partially filled, find the shape and the $k$-space dimensions of the Fermi surface, in terms of $\varepsilon_F$.

(b) Find the density of states, $D(\varepsilon)$, for this band. Note: the volume of an ellipsoid having principal radii $a$, $b$, and $c$ is $\dfrac{4\pi}{3}abc$.

(c) The unit cell dimensions for this crystal are $(a \times a \times c)$, with all angles right angles. Assume in this case that $c = a/3$. What are the dimensions of the reciprocal-space unit cell?

(d) For what electron density $(n = N/V)$ in this solid will the Fermi surface just touch the Brillouin zone boundary? Give your answer in terms of $a$. (Assume that [1] is an effective free-electron band; in other words we are neglecting any band-bending that would normally occur at the zone boundaries.)

(2)      For the two-dimensional net pictured below,

(a)  How many atoms are there per primitive unit cell?

(b)  Draw a primitive cell, and a pair of primitive vectors,  on the figure below.

(c)  On the same figure, draw a pair of primitive vectors for the reciprocal lattice, which correspond to your choice of direct-lattice primitive vectors.  (Be sure to label clearly for me which are the direct lattice vectors and which are the reciprocal vectors!)

(d) Sketch sets of lattice planes corresponding to the following:  (0,1) planes, (1,0) planes, and (4,1) planes.  (These should match your choice of vectors in (b).) Note: if the figure is too crowded, go ahead and make some or all on a separate sketch,  but keep the orientation the same so that I can understand.
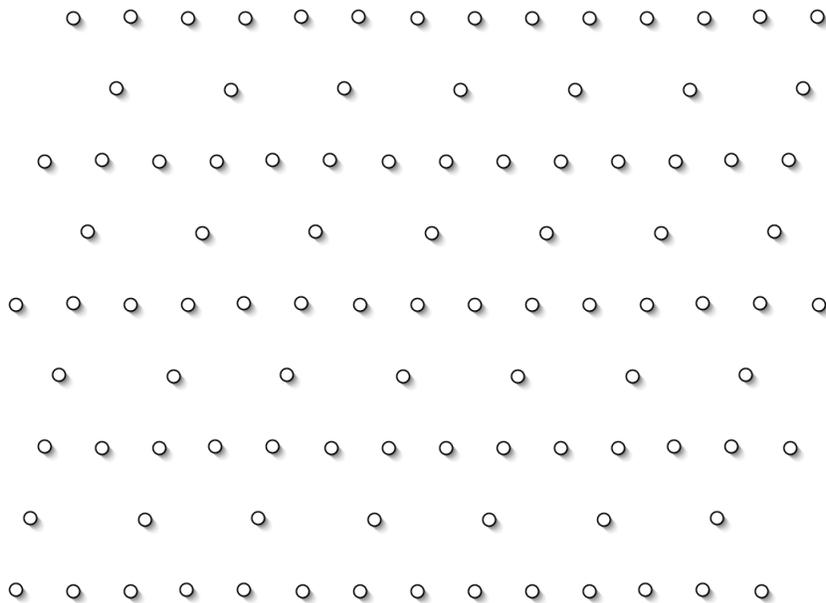
(3)     The Perovskite lattice of $CaTiO_3$ is pictured on p. 29 of the text.

(a)  How many atoms are there per unit cell?

(b)  Calculate the structure factor for x-ray scattering from this lattice, in terms of the three form factors: $f_{Ca}, f_{Ca}$, and $f_{Ca}$.  What is the lowest-angle reflection which has the maximum intensity value from your result (assuming the $f$'s are real, positive constants)?

(c) If you had completely arbitrary choice on the x-ray wavelength, what would be the largest x-ray wavelength which would still allow diffraction from the maximum-intensity line identified in (b)? [Answer in terms of the lattice constant $a$; numbers not needed.]

(4)    Consider a cubic lattice with a basis consisting of two identical atoms, one at the cube corner $(0, 0, 0)$, and one at the position $(a/4, a/4, 0)$, where $a$ is the cubic lattice constant. Suppose further that the potential seen by electrons in this lattice is simply a sum of identical delta functions, $A\delta(\vec{r} - \vec{R}_i)$, for each atom position $R_i$, with $A$ a constant.

(a) Describe the first Brillouin zone for this lattice.

(b) In the nearly-free electron model, sketch the energy vs. $k$ along the directions (100) and (001), for $k$ within the first Brillouin zone. Do this for the lowest energy band.

(c) Determine the magnitude of the energy gaps at the zone boundaries for the two directions plotted in (b), in terms of $A$.

(d) In general, the bands in the reduced zone scheme can be given by adding all possible $K$ vectors to $k$. Write down a general set of $K$ vectors, and use this to write a general expression for $\varepsilon$ vs. $k$ in the reduced zone scheme. (Do this for the free electron case, neglecting band gaps.)

(e) At $k = 0$ in the reduced-zone scheme, what are the four lowest free-electron energies, and what is the <u>degeneracy</u> of the bands crossing at $k = 0$ for each of these four energies?