Supplemental Problems for Chapter 2

1) Consider a lattice for which a = b = 4Å, c = 6Å, and $\alpha=\beta=\gamma=90°$.

(i) How many fourth nearest neighbors does each lattice site have?
(ii) How far away is the fourth nearest neighbors on this lattice, and in what directions are they?
(iii) Calculate the smallest angle between a vector pointing to a third nearest neighbor and a vector pointing to a fourth nearest neighbor.
(iv) Sketch two projections of this lattice, one along [100] and another along [001].
(v) Determine the lengths and directions of the reciprocal lattice vectors, a*, b*, and c*, and then sketch two projections of the reciprocal lattice, one along [100] and another along [001].
(vi) Calculate the angle between the [111] direction and the vector perpendicular to the (111) plane.
(vii) Find an equation for all possible d-spacings in this crystal.
(viii) Assuming that you record a diffraction pattern from this lattice using an X-ray wavelength of 1.54 Å, what are the diffraction angles (θ_{hkl}) and Miller indices of the first five Bragg diffraction peaks (these are the five with the smallest values of θ_{hkl})?
(this assumes knowledge of Bragg's Law, which is in Chapter 5)

2) In the cubic I lattice, each lattice point has eight near neighbors at a distance of $\sqrt{3}a/2$. How many sixth near neighbors does a lattice point have and how far away are they?

3) In rock salt (a cubic crystal), dislocations glide along {110}. Consider a crystal bound entirely by {100} faces. Along what directions would you expect to observe slip traces on the external surfaces of a deformed crystal? Another way of phrasing this question is, along what directions do the {110} planes in a cubic crystal intersect the {100} surfaces?

4) Consider an orthorhombic P lattice with the following dimensions: a = 14, b = 4, c = 5 Å.
(i) Sketch a projection of the direct lattice along [100] and the reciprocal lattice along [100]*.
(ii) What is the angle between the directions [010] and [010]*?
(iii) What is the angle between the [011] and [011]* direction?
(iv) Is the vector [011] perpendicular to the plane (011)?
(v) What is the angle between the (011) and (012) planes?

5) What is the conventional name for a cubic lattice with only one set of faces centered?

6) Consider a tetragonal crystal (a = 4.5 Å and c = 3.0 Å) with the following atomic positions occupied:
A atoms at (0,0,0) and (1/2, 1/2, 1/2)
B atoms at (0.3, 0.3,0), (0.7, 0.7,0), (0.8, 0.2,1/2), and (0.2, 0.8,1/2)
(i) What type of lattice does this structure have?
(ii) What is the basis?
(iii) Sketch a picture of the atoms on the (001) and (002) planes.
(iv) Sketch the (110) plane.
(v) What is the direction that connects the B atoms at (0.3, 0.3,0) and (0.7, 0.7,0)?

(vi) What is the sequence of atoms that occurs along this direction?
(vii) What are the distances from the A atoms at (1/2,1/2,1/2) to the surrounding B atoms?
(viii) What bond angle is formed by the atoms at (0.3, 0.3,0), (1/2, 1/2, 1/2), and (0.3, 0.3, 1)?

7) Consider a tetragonal I lattice, with lattice parameters a = 4 Å and c = 7 Å.
(i) Find a set of primitive lattice vectors and demonstrate that there is one lattice point per cell using this set.
(ii) Sketch the direct lattice and label the points, first with the conventional lattice vectors and then with the primitive vectors.
(iii) Find primitive and conventional reciprocal lattice vectors; sketch the reciprocal lattice and label the points, first with the conventional vectors and then with the primitive vectors.
(iv) Is the [101] direction perpendicular to the (101) plane? (the indices are with respect to the conventional lattice)
(v) What is the angle between the (102) and (010) planes?
(vi) Write a general expression (involving a, c, h, k, and l) for the interplanar spacings of this lattice.

8) What Bravais lattice arises when the cF lattice is elongated parallel to one of the lattice vectors? Please use a sketch of the lattice to illustrate your answer.

9) Which of the following planes belong to the [111] zone?
$(2\bar{3}1)$, $(\bar{3}\bar{1}3)$, $(\bar{1}\bar{1}2)$, $(\bar{2}21)$

10) Specify 8 plane that belong to the [112] zone with $-3 \le h, k, l \le +3$

11) Consider an orthorhombic P lattice with the following dimensions: a = 10, b = 3, c = 4 Å.

(i) Sketch a projection of the direct lattice along [001] and the reciprocal lattice along [001]*. Extend the lattices at least to the range of $-2 \le u, v \le 2$ and $-2 \le h, k \le 2$. Please make sure that you draw them to scale and indicate the scale on the figure.

(ii) What is the angle between the directions [010] and [010]*?

(iii) What is the angle between the [011] and [011]* direction?

(iv) Is the vector [011] perpendicular to the plane (011)?

(v) What is the angle between the (011) and (012) planes?

(vi) What are the interplanar spacings for the (011) and (012) planes? (d_{011} and d_{012})

(vii) In an X-ray diffraction experiment, using Cu kα radiation (λ = 1.54 Å), at what angles (θ) are the first five Bragg diffraction peaks observed (the five peaks with the smallest values of θ)?

10) Given lattice vectors:

$$\vec{a} = a\left(\frac{\sqrt{3}}{2}\hat{x} - \frac{1}{2}\hat{y}\right), \quad \vec{b} = a\hat{y}, \quad \vec{c} = c\hat{z}$$

(i) Show that these are valid Bravais lattice vectors.
(ii) Compute the volume of the cell defined by these vectors.
(iii) What is than angle between $\vec{a}$ and $\vec{b}$?
(iv) Sketch the direct lattice, projected along [001].
(v) Sketch the reciprocal lattice, in the same projection and orientation.
(vi) What is the distance from (0,0,0) to (1,1,1) in this cell?
(vii) Write a formula for the interplanar spacings of the planes in this lattice.